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A PROGRAM FOR A LOCALLY-PARAMETRIZED CONTINUATION PROCESS.(U)
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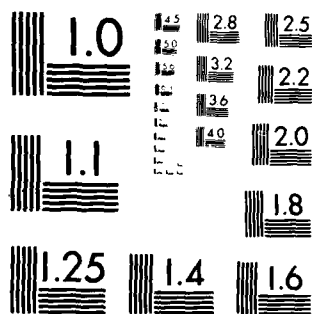
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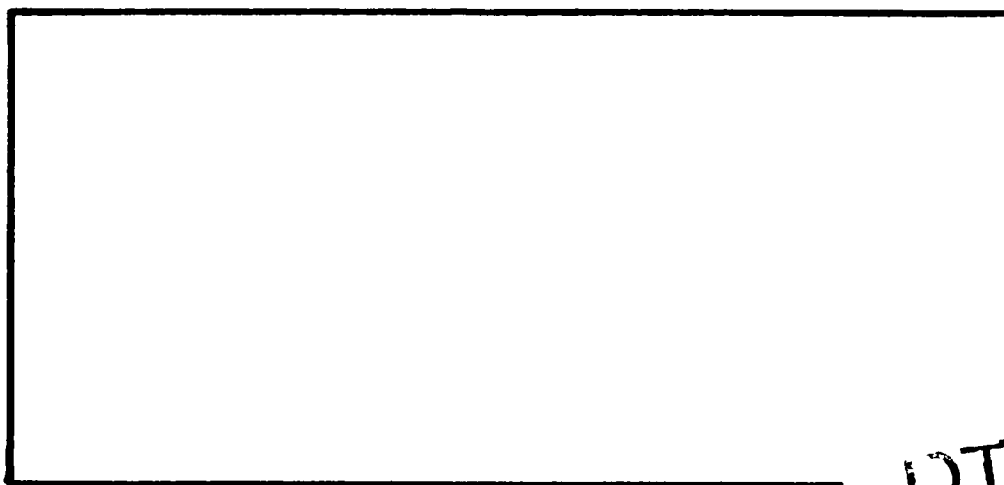
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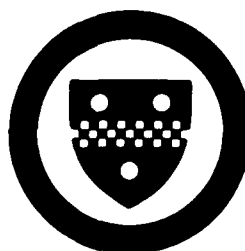


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A Program for a Locally-Parametrized
Continuation Process^{*)}

by

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1. INTRODUCTION

The study of many equilibrium phenomena leads to non-linear equations which involve a number of intrinsic parameters. Interest then centers rarely on the determination of a few specific solutions of the equations for fixed parameter values but rather on an assessment of the behavior of these solutions under general variations of the parameters. For example, in structural analysis the parameters may characterize load points and load directions, material properties, geometrical data, etc. The set of all solutions and associated parameter values has been called the equilibrium surface of the structure (see eg. [31]). This equilibrium surface provides considerable insight into the behavior of the structure and the stability properties (see eg. [23], [32] for further discussions and various examples). From a numerical viewpoint the question then is to analyze computationally the shape and characterize particular features of this equilibrium surface.

In nonlinear mechanics the principal tools for such a computational analysis are the so-called incremental methods. These procedures were developed more or less independently in the engineering literature. But they are now also recognized to be closely related to the continuation methods used for some time in mathematics in general and in numerical analysis in particular. The literature in this area is extensive: we refer only to [21] for a discussion about the connection between incremental approaches for structural problems and continuation methods, to [8] for a historical overview of uses of continuation techniques in mathematics and to [2], [35] for some literature survey of numerical aspects of continuation methods.

Not surprisingly there are differences between the methods used in structural engineering and numerical analysis and neither is directly suited to the analysis of an equilibrium surface. In the numerical analysis liter-

ature continuation methods are usually considered only as tools for determining a specific solution y^* of a given nonlinear operator equation $Gy = 0$. For this the equation is imbedded into a one-parameter family $H(y,t) = 0$ which has a solution $y = y(t)$ for each fixed t in some interval, say, $0 \leq t \leq 1$. (See eg. [15] for a survey of such imbeddings.) If $y(t)$ depends continuously on t and satisfies $y(0) = y^0$ and $y(1) = y^*$, where y^0 is a known point, then the numerical process constructs a sequence of points in the proximity of the path $y(t)$, $0 \leq t \leq 1$, starting at y^0 and ending at the desired point y^* . On the other hand, in structural mechanics incremental methods usually are designed to follow numerically a specific load curve parametrized by a load intensity. Hence, while in the imbedding approach the parameter is essentially artificial, in the incremental procedures it has an intrinsic meaning for the application, and, even more importantly, there is no longer a fixed endpoint which is the aim of the computation, but the load curve itself is of interest.

For a numerical analysis of a given equilibrium surface we need to consider continuation-methods in a broader sense as a collection of numerical procedures for completing at least the following three basic tasks:

- (i) Follow numerically any curve on the surface specified by a particular combination of parameter values with one degree of freedom.
- (1.1) (ii) On any such curve determine the exact location of target points where a given state variable has a specified value.
- (iii) On such a curve identify and compute exactly the critical points where stability may be lost.

Beyond this various more special tasks may arise as, for example, the following ones:

- (iv) From any one of the critical points determined under (iii) follow a path in the critical boundary.
- (1.2) (v) On any one of the curves (i) determine the location of bifurcation points and the paths intersecting at that point.

Methods which are either directly applicable or can be readily adapted to completing these various tasks have been proposed by various authors. In particular, for (i) the literature is very large and we refer here only to the mentioned surveys [2], [35]. Methods relating to (iii) were described, for instance, in [1], [20], [22], [33], [34], and for (iv) and (v) we refer to [28] and [10], [25], respectively, where also further references are given.

So far only a few library programs for performing these various tasks have been published. Without claim for completeness we mention here [14], [38]. Each one of these programs has the objective of computing a specified solution curve of a nonlinear equation by a continuation approach along the lines sketched above. In this paper, we present a new library package specifically written with the objective of completing the three basic tasks (1.1) (i), (ii), (iii). The package can be expanded to incorporate facilities for (1.2) (iv), (v), but this will not be addressed here. The package is based on the continuation approaches introduced in [26], [27] and incorporates some of the concepts of steplength determination discussed in [7]. At the same time, new techniques of parameter adaptation are utilized here based on a prediction of changes in the curvature of the continuation path.

As with all programming packages further improvements are possible. For example, it is planned to introduce an automatic first step selection and a function-scaling option. Special versions incorporating facilities for the tasks (1.2) are also being designed. But since all these changes are built on the present package the presentation of a documentation of PITCON in its basic form appeared desirable and justified.

G and K of (2.3) are provided for by the user. In other words, we may write (2.3) as one equation

$$(2.4) \quad Fx \approx 0$$

with a user-specified mapping $F: R^n \rightarrow R^{n-1}$. Note, however, that in this underdetermined equation (2.4) no one variable is explicitly identified as continuation variable as is typical in the incremental and continuation methods mentioned in the introduction.

We assume here that the given mapping F has the following properties:

- (i) F is continuously differentiable on R^n .
- (2.5) (ii) The derivative $DF(x)$ of F is locally lipschitzian on R^n .
- (iii) The regularity set $R(F) = \{x \in R^n; \text{rank } DF(x) = n-1\}$ is non-empty and therefore an open subset of R^n .

From (2.5) it follows (see [26]) that the tangent map specified by

$$(2.6) \quad T: R(F) \rightarrow R^n, \quad DF(x)Tx = 0, \quad ||Tx||_2 = 1, \quad \det \begin{pmatrix} DF(x) \\ (Tx)^T \end{pmatrix} > 0$$

is uniquely determined and locally lipschitzian on $R(F)$. Furthermore, (2.5) implies that the regular solution set $E(F) \cap R(F)$ of F is either empty or a one-dimensional C^1 -manifold in the open set $R(F)$. Our objective is to determine numerically a non-empty connected component E^* of $E(F) \cap R(F)$. It is well-known (see eg. [17]) that such a component E^* is diffeomorphic either to the circle or to some interval (that is, some connected subset) of R^1 . Hence, E^* is uniquely determined by any one of its points $x^0 \in E(F) \cap R(F)$

and we denote this by writing $E^*(F, x^0)$. Note that for any $x^1 \in E^*(F, x^0)$ we have $E^*(F, x^1) = E^*(F, x^0)$.

A parametrization by arclength of $E^*(F, x^0)$ is a solution of the initial value problem

$$(2.7) \quad \dot{x} = Tx, \quad x(0) = x^0.$$

Note that, since T is locally Lipschitzian, (2.7) has a unique solution which cannot terminate inside $R(F)$. Evidently standard ODE-solvers may be applied to solve (2.7) numerically. This has been pursued for some time in the literature (see eg. [3], [6], [13], [37]). Independent of this, the choice of the arclength for the parametrization of $E^*(F, x^0)$ has been proposed by many authors. Notably H. B. Keller and his co-workers (see eg. [10], [11]) have advocated this choice for some time. It is also the basis of incremental procedures given in [5], [29] and has been more or less implicit in various papers in the field.

Our programs here are based more generally on the structure of $E^*(F, x^0)$ as a one-dimensional manifold and use a local parametrization at each point computed along $E^*(F, x^0)$. A natural class of such local parameters are the n components of the vector x . We call a process based on this choice of parametrization a locally-parametrized continuation method.

3. OUTLINE OF THE PROCESS AND BASIC STEPS

As noted before, our objective is to determine numerically a non-empty component $E^*(F, x^0)$ of the regular solution set $E(F) \cap R(F)$. For the discussion it is useful to consider a parametrization by arclength of $E^*(F, x^0)$, that is, a function $x: J \rightarrow E^*(F, x^0)$ which maps some interval $J \subset \mathbb{R}^1$ diffeomorphically onto some open subset of $E^*(F, x^0)$ such that $\|\dot{x}(s)\|_2 = 1$ for $s \in J$. We may assume also that $x(0) = x^0$, $0 \in J$.

The process described here belongs to the class of predictor-corrector continuation methods. Starting from x^0 it produces a sequence of approximations $x^k \doteq x(s_k)$, $k = 0, 1, \dots$, corresponding to some sequence $0 = s_0 < s_1 < s_2 < \dots$ of arclength values. Note, however, that in general the values s_1, s_2, \dots are only approximately computable and are of limited interest in most applications.

In our program the principal steps performed during one continuation step are as follows:

1. Initialization.
2. Check for and computation of target point, if desired.
3. Calculation of tangent vector and determination of new local continuation parameter.
- (3.1) 4. Check for and computation of limit point, if desired.
5. Steplength computation.
6. Computation of predicted point and corrector iteration.
7. Storage of data and return.

The sequencing of these steps is dictated by the data-flow. For the description of the details it will be advantageous not to adhere to this

sequence. Instead, in the remainder of this section, we discuss the basic steps 3. and 6. Then the next section introduces the new steplength computation used in step 5. and section 5 covers steps 2. and 4. The data-handling steps 1. and 7. should be self-explanatory from the documentation of the program itself.

Let e^1, \dots, e^n be the natural basis vectors of R^n . Then it is readily verified that (see eg. [26])

$$(3.2) \quad \det \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix} = [(e^i)^T Tx] \det \begin{pmatrix} DF(x) \\ (Tx)^T \end{pmatrix}, \quad \forall x \in R(F), \quad i = 1, \dots, n,$$

where the matrix occurring on the right is non-singular. Hence, for any index i , $1 \leq i \leq n$, such that $(e^i)^T Tx \neq 0$, the solution $v \in R^n$ of the linear system

$$(3.3) \quad \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix} v = e^n$$

is uniquely defined. Evidently, then

$$(3.4) \quad Tx = \sigma \frac{v}{\|v\|_2},$$

and, in line with (2.6), we should set

$$(3.5) \quad \sigma = \text{sign}(v^T e^i) \text{sign} \det \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix}.$$

As long as the solution path remains completely in $R(F)$ this is satisfactory.

But frequently in applications we may encounter a bifurcation point $x^* \notin R(F)$ where several solution paths terminate. For example, using arclength representations we may find solutions $x^j: J_j \subset \mathbb{R}^1 \rightarrow R(F)$, $j = 1, \dots, 4$, for which $x^j(s)$ tends to x^* when s tends to one of the endpoints of J_j . Moreover, it often happens that there are pairs of these solutions, say, x^1 and x^2 for which $\lim \dot{x}^1(s) = -\lim \dot{x}^2(s)$ at x^* , (see Fig. 1). In other words, if we disregard the direction of the solutions, they appear to form one smooth curve through x^* . In such a case, when the process moves along x^1 toward x^* it usually "jumps" over x^* onto x^2 . Then, unless we reverse the sign of σ in (3.4) the tangent will again point toward x^* and the process reverses direction.

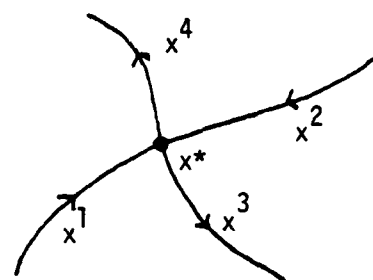


Figure 1

In order to avoid this problem suppose that the point x in (3.4) is the k -th approximation computed along the curve. Then σ is determined as follows

$$(3.6) \quad \sigma = \begin{cases} \text{dir}, & \text{if } k = 0 \\ +1, & \text{if } \text{sign } v^T e^i = \text{sign}(Tx^{k-1})^T e^i \\ -1, & \text{otherwise} \end{cases}$$

where dir is a user specified direction at the starting point. By comparing this value of σ with that of (3.5) we can detect if the process did jump over a bifurcation point of odd multiplicity. Obviously, bifurcation points of even multiplicity cannot be found this way.

Once the tangent Tx^k has been obtained we determine the indices j_1 and j_2 of the largest and second largest component of Tx^k in modulus,

respectively. The relation (3.2) certainly suggests that the index i_k , $1 \leq i_k \leq n$, of the new local continuation variable be set equal to j_1 . However, if we are approaching a limit point in the j_1 -th variable then this choice may be disadvantageous. Accordingly, if the following three conditions are simultaneously satisfied

$$\begin{aligned}
 & \text{(i)} \quad |(e^{j_1})^T T x^k| < |(e^{j_1})^T T x^{k-1}|, \\
 (3.7) \quad & \text{(ii)} \quad |(e^{j_2})^T T x^k| > |(e^{j_2})^T T x^{k-1}|, \\
 & \text{(iii)} \quad |(e^{j_2})^T T x^k| \geq \mu |(e^{j_1})^T T x^k|,
 \end{aligned}$$

with a fixed μ , $0 < \mu < 1$, then we set $i_k = j_2$. Of course, if we don't have a previous tangent vector this check has to be bypassed. The new continuation index i_k will be used for the computation of the next point x^{k+1} and its tangent $T x^{k+1}$. For the tangent computation at x^0 a continuation index is assumed to be given by the user.

With the tangent $T x^k$ and the steplength $h_k > 0$ determined by the steplength algorithm of section 4 we compute now the predicted point $\hat{x}^k = x^k + h_k T x^k$. Then any appropriate iterative method for the solution of the augmented equation

$$(3.8) \quad \hat{F}x \equiv \begin{pmatrix} Fx \\ (e^{i_k})^T (x - \hat{x}^k) \end{pmatrix} = 0$$

starting from \hat{x}^k may be used as a corrector process. In the program we use either the regular Newton method or its modified form in which the Jacobian at the starting point is held fixed.

Let $y^0 = \hat{x}^k, y^1, y^2, \dots$ be the iterates produced in this way. The process has to incorporate provisions for monitoring the convergence and for aborting the iteration as soon as divergence is suspected. In the program non-convergence is declared if any one of the following three conditions is true

$$\begin{aligned}
 & \text{(i)} \quad ||\hat{F}y^j|| \geq \theta ||\hat{F}y^{j-1}|| \quad \text{for some } j \geq 1, \\
 (3.9) \quad & \text{(ii)} \quad ||y^j - y^{j-1}|| \geq \theta ||y^{j-1} - y^{j-2}|| \quad \text{for some } j \geq 2, \\
 & \text{(iii)} \quad j \geq j_{\max}.
 \end{aligned}$$

For the constant θ we use $\theta = 1.05$ except in the first check of (3.9) (i) where $\theta = 2$ is chosen. The maximal iteration count j_{\max} depends on the method. For the regular Newton process we set $j_{\max} = 10$ and double this for the modified method. In the case of non-convergence the predictor step is reduced by a given factor, for example 1/3, unless the resulting step is below a given minimal steplength.

Convergence is declared if either one of the two conditions holds for an iterate:

$$\begin{aligned}
 & \text{(i)} \quad ||\hat{F}y^j|| \leq 8 \epsilon_{\text{mach}} \quad \text{for some } j \geq 0, \\
 (3.10) \quad & \text{(ii)} \quad (||\hat{F}y^j|| \leq \epsilon_{\text{abs}}) \quad \text{and} \quad (||y^j - y^{j-1}|| \leq \epsilon_{\text{abs}} + \epsilon_{\text{rel}} ||y^j||) \quad \text{for some } j \geq 1.
 \end{aligned}$$

The tolerances $\epsilon_{\text{abs}}, \epsilon_{\text{rel}}$ are user specified and ϵ_{mach} is the smallest floating point number such that $1. = 1. + \epsilon_{\text{mach}}$. In both tests (3.9) and (3.10) the maximum norm is used.

4. THE STEPLENGTH ALGORITHM

For the points x^k , $k = 0, 1, \dots$, approximating the continuation curve $x: J \rightarrow E^*(F, x^0)$ the achievable error $||x^k - x(s_k)||$ is solely determined by the termination criterion (3.10) of the corrector process. In contrast to this the standard ODE-solvers involve a corrector equation obtained by extrapolation for which the solutions are not, in general, on the exact curve. As a consequence the available error for the ODE-solvers depends on the history of the process up to that point, and this in turn has a strong influence on the step-selection. On the other hand, for our continuation process any step $h_k > 0$ along the Euler line is acceptable in principle if only the corrector converges from the predicted point \hat{x}^k . Moreover, in [26] it was shown that any compact segment of the continuation curve in $R(F)$ has an ϵ -neighborhood for some $\epsilon > 0$ in which Newton's method will converge to the curve.

This suggests that we estimate the radius of convergence of the corrector process at the computed points and extrapolate these radii to the next point about to be determined. In practice the estimate of a convergence radius at some continuation point would have to be based on the corrector iterates which led to that point. Unfortunately, as was proved in [7], this represents insufficient information for obtaining such an estimate. On the other hand, an approach was presented in [7] which allows for an assessment of the convergence quality of the particular sequence of corrector iterates.

For details of this approach we refer to the cited article. In brief, let $\{y^i\}$ be a given sequence with limit y^* generated by an iterative process and denote the errors by $e_i = ||y^i - y^*||$, $i = 0, 1, \dots$. The definition of any convergence measure is based on a hypothetical model of the behavior of the errors. For example, if $\{y^i\}$ converges linearly it is reasonable to assume that

$$(4.1) \quad 0 \leq e_{i+1} \leq \lambda e_i, \quad i = 0, 1, \dots$$

with some constant λ , $0 < \lambda < 1$, depending on $\{y^i\}$. Suppose now that the process was terminated with the iterate y^{i^*} . Then

$$(4.2) \quad \tilde{\lambda} = \tilde{\omega}^{1/(i^*-1)}, \quad \tilde{\omega} = \frac{||y^{i^*} - y^{i^*-1}||}{||y^{i^*} - y^0||}, \quad i^* \geq 2,$$

represents a computable estimate of λ .

In the setting of our continuation process suppose now that the y^i , $i = 0, 1, \dots$, are the corrector iterates leading from the current predicted point $\hat{x}^k = y^0$ to the new continuation point $x^{k+1} = y^{i^*}$. Then

$$(4.3) \quad \delta_k = ||\hat{x}^k - x^{k+1}|| = ||y^0 - y^{i^*}||$$

is the correction-distance. For the modified Newton method the convergence is indeed linear, and a reasonable aim in the construction of the steps along the curve is to ensure that the number of corrector iterates remains about constant. In other words, we aim at taking always, say, m^* corrector steps. Hence, under the heuristic assumption that the error model (4.1) remains valid for some interval of starting errors e_0 around δ_k , we should have begun with an "ideal starting error" $\delta_k^* = \theta_k \cdot \delta_k$ such that

$$(4.4) \quad \tilde{\lambda}^{m^*} \delta_k^* = \tilde{\lambda}^{i^*} \delta_k$$

and therefore

$$(4.5) \quad \theta_k = \bar{\lambda}^{i^*-m^*} \equiv \bar{\omega}^{(i^*-m^*)/(i^*-1)}.$$

In our program we use $m^* = 10$ for the modified Newton method and enforce always that $0.125 \leq \theta_k \leq 8$.

This technique is also readily applicable for Newton's method. In [7] two different hypothetical error models for the Newton process were discussed. Here we use only one of these models, namely the one arising in the attraction theorem formulated in [24]. In essence, under certain conditions about the equation and the desired limit y^* of the Newton process there exists a radius $r^* > 0$ such that for any starting point y^0 in the ball $B(y^*, r^*)$ the relative errors $\varepsilon_i = e_i/r^*$, $i = 0, 1, \dots$, satisfy

$$(4.6) \quad 0 \leq \varepsilon_{i+1} \leq \phi(\varepsilon_i), \quad i = 0, 1, \dots, \quad \phi(t) = \frac{t^2}{3-2t}, \quad 0 \leq t \leq 1.$$

The radius r^* depends on global information about the equation and is not accessible. If $0 < \varepsilon_0 < 1$ and the $\{\varepsilon_i\}$ satisfy (4.6) then we have

$$(4.7) \quad \varepsilon_i \leq \eta_i \equiv \phi^i(\eta_0) \equiv \frac{3}{1 + 2 \cosh 2^i \alpha}, \quad i = 0, 1, \dots, \quad \eta_0 = \varepsilon_0,$$

where α is the unique positive solution of

$$(4.8) \quad \psi(\alpha) = \eta_0, \quad \psi(\alpha) = \frac{3}{1 + 2 \cosh \alpha}.$$

Moreover, for any ω , $0 < \omega < 1$, and $i^* \geq 2$ the equation

$$(4.9) \quad \frac{1}{\psi(\alpha)} \phi^{i^*-1}(\psi(\alpha)) \equiv \frac{1 + 2 \cosh \alpha}{1 + 2 \cosh 2^{i^*-1} \alpha} = \omega$$

has a unique solution $\alpha > 0$.

Now suppose that $\{y^i\}$ denotes the sequence of Newton iterates and that the process was terminated at y^{i^*} . As in the linear case we use the approximation

$$(4.10) \quad \tilde{\omega} = \frac{||y^{i^*} - y^{i^*-1}||}{||y^{i^*} - y^0||} \doteq \frac{e_{i^*-1}}{e_0} = \frac{\varepsilon_{i^*-1}}{\varepsilon_0} \leq \frac{\eta_{i^*-1}}{\eta_0}$$

and compute with this $\tilde{\omega}$ the solution $\tilde{\alpha}$ of (4.9) which gives the estimate $\tilde{\eta}_0 = \psi(\tilde{\alpha})$ of ε_0 . Now we proceed as before and obtain the factor

$$(4.11) \quad \theta_k^* = \frac{\delta_k^*}{\delta_k} = \frac{\tilde{\eta}_0'}{\tilde{\eta}_0}$$

for the ideal starting error by determining the unique solution $\tilde{\eta}_0'$, $0 < \tilde{\eta}_0' < 1$, of

$$(4.12) \quad \phi^{m^*}(\tilde{\eta}_0') = \phi^{i^*}(\tilde{\eta}_0).$$

Since the iterates ϕ^i are explicitly known the various equations are not difficult to solve numerically. However, for the computation it is more advantageous to introduce a least squares fit of θ_k as a function of $\tilde{\omega}$ for all relevant values of i^* . In the program we use $m^* = 4$ and the approximations for θ_k given in Table 1. Note that as before we restrict θ_k to the interval $0.125 \leq \theta_k \leq 8$.

i^*	$\tilde{\omega} \in [a, b]$		θ_k
	a	b	
2	0.8735115	1	1
	0.1531947	0.8735115	$0.9043128 - 0.7075675 \ln \omega$
	0.03191815	0.1531947	$-4.667383 - 3.677482 \ln \omega$
	0	0.03191815	8
3	0.4677788	1	1
	0.6970123(-3)	0.4677788	$0.8516099 - 0.1953119 \ln \omega$
	0.1980863(-5)	0.6970123(-3)	$-4.830636 - 0.9770528 \ln \omega$
	0	0.1980863(-5)	8
4	0	1	1
5	0.3339946(-10)	1	$1.040061 + 0.03793395 \ln \omega$
	0	0.3339946(-10)	0.125
6	0.1122789(-8)	1	$1.042177 + 0.04450706 \ln \omega$
	0	0.1122789(-8)	0.125
≥ 7	0	1	0.125

Table 1

We turn now to the algorithm for the determination of the steplength $h_k > 0$ along the Euler line $\pi(t) = x^k + t T x^k$ used for the prediction. In order to estimate the distance between $\pi(t)$ and the exact curve $x = x(s)$ we introduce the quadratic Hermite-Birkhoff interpolation polynomial

$$(4.13) \quad q(t) = x^k + t T x^k + \frac{1}{2} t^2 w^k, \quad w^k = \frac{1}{\Delta s_k} (T x^k - T x^{k-1}), \quad \Delta s_k = \|x^k - x^{k-1}\|_2$$

for which

$$(4.14) \quad q(0) = x^k, \quad q'(0) = T x^k, \quad q'(-\Delta s_k) = T x^{k-1}.$$

Since

$$(4.15) \quad w^k = \int_0^1 x''(s_k - \sigma \Delta s_k) d\sigma = x''(s_k - \tilde{\sigma} \Delta s_k), \quad 0 < \tilde{\sigma} < 1,$$

the quantity

$$(4.16) \quad \|w^k\|_2 = \frac{2}{\Delta s_k} |\sin \frac{1}{2} \alpha_k|, \quad \alpha_k = \arccos ((T x^k)^T T x^{k-1})$$

represents an approximation of the curvature of the exact point at some point between $x(s_{k-1})$ and $x(s_k)$.

It is tempting to derive from q a prediction of the curvature to be expected during the next continuation step. However, a closer computation shows that the value of the curvature of q assumes its maximum $\|w^k\|_2 / \cos^2 \frac{1}{2} \alpha_k$ at $t = -\frac{1}{2} \Delta s_k$ and that for increasing t this value decreases rapidly. For example, at $t = 0$ the curvature of q equals only $\|w^k\|_2 |\cos \frac{1}{2} \alpha_k|$ and for positive t no reasonable predictive information can be gained this way.

The relation (4.15) suggests the use of the simple linear extrapolation

$$(4.17a) \quad \gamma_k^{\text{tent}} = \|w^k\|_2 + \frac{\Delta s_k}{\Delta s_k + \Delta s_{k-1}} (\|w^k\|_2 - \|w^{k-1}\|_2)$$

for a prediction of the curvature during the next continuation step. However, this value may become negative and accordingly we use instead

$$(4.17b) \quad \gamma_k = \max(\gamma_{\min}, \gamma_k^{\text{tent}})$$

with a given small $\gamma_{\min} > 0$.

Most of the data discussed so far are sketched in Figure 2. In order to derive a formula for the desired predictor step h_k we note that

$$(4.18) \quad \|q(t) - \pi(t)\|_2 = \frac{1}{2} t^2 \|w^k\|_2$$

represents an estimate of the distance between the Euler line and the exact curve. In fact, for smooth curves the error of this estimate is asymptotically of order three in $\max(|t|, \Delta s_k)$ as this quantity tends to zero. Hence, if we want this distance to be at most equal to a tolerance $\epsilon > 0$ then we should choose the next step as

$$(4.19) \quad t = \sqrt{\frac{2\epsilon}{\|w^k\|_2}}.$$

It is natural to replace the curvature $\|w^k\|_2$ by the predicted value γ_k of (4.17) and to relate the tolerance ϵ to the "ideal starting error" δ_k^* obtained earlier. As Figure 2 indicates it is unreasonable to expect $\epsilon > \Delta s_k$. Hence, we use instead

$$(4.20) \quad \epsilon_k = \begin{cases} \epsilon_{\min} \Delta s_k & \text{if } \delta_k^* \leq \epsilon_{\min} \Delta s_k \\ \Delta s_k & \text{if } \delta_k^* \geq \Delta s_k \\ \delta_k^* & \text{otherwise} \end{cases}$$

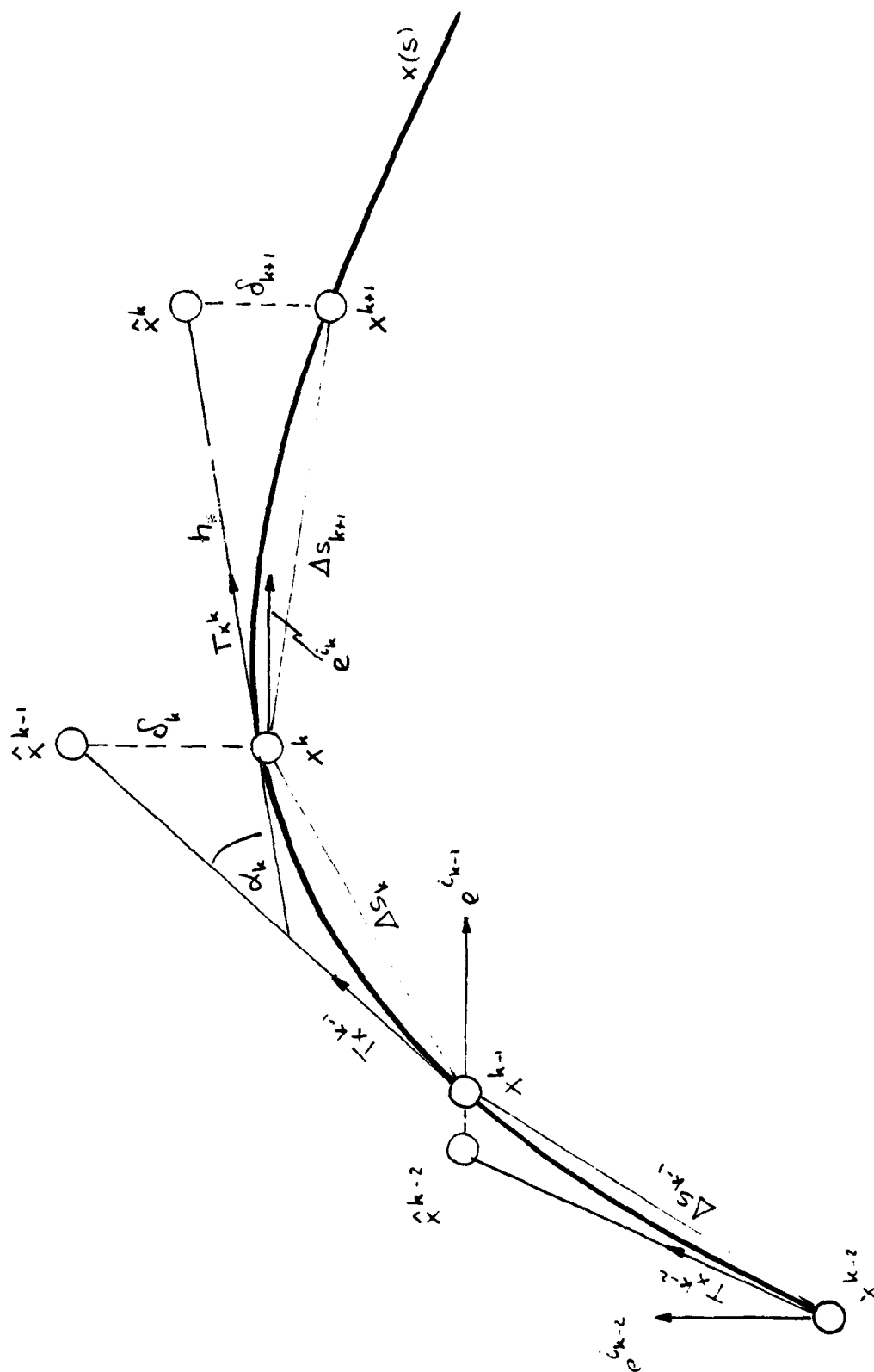


Figure 2

with a small $\epsilon_{\min} > 0$, e.g., $\epsilon_{\min} = 0.01$. Then a tentative predicted step is given by

$$(4.21) \quad h_k^{(1)} = \sqrt{\frac{2\epsilon_k}{\gamma_k}}.$$

From the form (3.8) of the augmented equation we see that the corrector iterates remain in a hyperplane perpendicular to the basis vector e^i_k through the predicted point. Then Figure 2 suggests that we adjust the predicted steplength h_k so as to ensure that h_k will be approximately equal to Δs_{k+1} . There is no need to enforce this too rigidly. It suffices to define a new tentative step by the requirement

$$(e^i)^T \pi(h_k^{(2)}) = (e^i)^T q(h_k^{(1)})$$

whence,

$$(4.22) \quad h_k^{(2)} = h_k^{(1)} \left[1 + \frac{h_k^{(1)}}{2\Delta s_k} \left(1 - \frac{(e^i)^T T x^{k-1}}{(e^i)^T T x^k} \right) \right].$$

This formula may involve subtractive cancellation and has to be evaluated in double precision.

The final value h_k of the steplength is now obtained from $h_k^{(2)}$ by enforcing three different bounding requirements. First of all, if the previous continuation step from x^{k-1} to x^k was obtained only after a failure of the correction process and a corresponding reduction of the predicted step, then we should not allow h_k to exceed Δs_k . Secondly, as in the ODE solvers we need to control both the relative growth and the absolute size of the pre-

dicator step. Thus, we require that

$$(4.23) \quad \frac{1}{\kappa} \Delta s_k \leq h_k \leq \kappa \Delta s_k, \quad h_{\min} \leq h_k \leq h_{\max}$$

where κ is some factor, say, $\kappa = 3$, and h_{\min}, h_{\max} depend on the machine as well as the requirements of the problem. It should be obvious how the final step h_k is obtained from $h_k^{(2)}$ on the basis of these restrictions.

5. THE COMPUTATION OF TARGET AND LIMIT POINTS

By generating a sequence of solution points on a given curve, the continuation process reveals the shape of the curve, but there are often other items of interest that need to be studied as well. Our program is designed to pause during the continuation steps in order to seek out special points that the user has requested, namely, target and limit points.

A target point $x \in E^*(F, x^0)$ is a point on the solution curve for which the component $x_i = (e^i)^T x$ with given index $i = IT$ has a prescribed value $\bar{x}_i = XIT$. Limit or turning points with respect to a given index $i = LIM$ are points $x \in E^*(F, x^0)$ where the i -th component $(e^i)^T Tx$ is zero. More specifically, since it is computationally unreasonable to attempt to compute zeroes of even order, we are concerned only with limit points on the continuation curve where $(e^i)^T Tx(s)$ changes sign.

It might be mentioned that bifurcation points represent another interesting, special class of points. But in that case we are not only interested in the specific location of the point but also in the solution curves that branch off from it. This is exactly the task (1.2) (v) listed earlier. The corresponding procedures (loc. cit.) would add considerably to the complexity of our program, and, since their utility tends to be of a more specialized nature, it was decided not to cover task (1.2) (v) (nor (1.2) (iv)) in the present program.

As indicated before, the determination of a target or limit point represents an interruption in the normal flow of the continuation program. After at least one step has been taken, the program has available an old point x^{k-1} , a new point x^k and the tangent vector Tx^{k-1} . Normally, then we turn to the computation of Tx^k , of the new steplength, and finally of the next point x^{k+1} . But if the index IT or LIM is non-zero then these

computations are postponed for the search of a target or limit point, respectively. We discuss these cases separately:

Target points: Suppose that a non-zero value of $i = IT$ and associated value $\bar{x}_i = XIT$ have been given. If \bar{x}_i lies between $(e^i)^T x^{k-1}$ and $(e^i)^T x^k$, then it is assumed that a solution point $x \in E^*(F, x^0)$ with $(e^i)^T x = \bar{x}_i$ is nearby. In this case a point

$$(5.1) \quad y(t) = (1-t)x^{k-1} + tx^k, \quad 0 \leq t \leq 1,$$

on the secant between x^{k-1} and x^k is determined such that $(e^i)^T y(t) = \bar{x}_i$. Now with the augmenting equation $(e^i)^T x = \bar{x}_i$ the corrector process is applied, and, if it terminates successfully the resulting point is taken as the desired target. Otherwise, a failure is indicated for the target routine. In either case, the routine returns and on the next call the continuation loop will pick up from where it was interrupted. Note that in effect the target routine uses the IT -th variable for the local parametrization of the curve between x^{k-1} and x^k . This may be an inferior choice of parameter for the corrector but it allows us to enforce that the resulting target point $x \in E^*(F, x^0)$ indeed satisfies $(e^i)^T x = \bar{x}_i$. Clearly, for very large continuation steps we have no guarantee that all target points will be detected or that a target computation will succeed. Thus, the utility of the target routine will depend on the maximal allowed stepsize that has been chosen.

Limit points: If the limit point index $i = LIM$ is non-zero, then a limit point determination is carried out after a target point search has been successfully or unsuccessfully completed, provided it was called for at all.

Recall that we still have as current information the vectors x^{k-1} , x^k , and Tx^{k-1} . Now the new tangent Tx^k is evaluated and if $\text{sign}(e^i)^T Tx^{k-1} \neq \text{sign}(e^i)^T Tx^k$ for $i = \text{LIM} (\neq 0)$ then a limit point search is begun. For this the index \hat{i} of the largest component in modulus of the secant direction $x^k - x^{k-1}$ is chosen as a local parametrization of the curve between x^{k-1} and x^k . More specifically, suppose that $x: [s_{k-1}, s_k] \rightarrow E^*(F, x^0)$ represents the segment of the curve between x^{k-1} and x^k . Then \hat{i} is assumed to be the index of a local coordinate for which there exists a bijective parameter transformation $\phi: [0, 1] \rightarrow [s_{k-1}, s_k]$ such that $(e^{\hat{i}})^T y(t) = (e^{\hat{i}})^T x(\phi(t))$, $0 \leq t \leq 1$, where $y(t)$ is defined by (5.1).

Hence, we may consider the function

$$(5.2) \quad g: [0, 1] \rightarrow \mathbb{R}^1, \quad g(t) = (e^{\hat{i}})^T Tx(\phi(t)), \quad 0 \leq t \leq 1,$$

and our problem is to determine a zero of g . Since by assumption $\text{sign } g(0) \neq \text{sign } g(1)$, a rootfinder of the Dekker-Brent type can be applied. For the evaluation of $g(t)$ we use the augmenting equation $(e^{\hat{i}})^T x = (e^{\hat{i}})^T y(t)$ and apply the corrector process with $y(t)$ as starting point. If it terminates successfully with some x then Tx can be evaluated and we set $g(t) = (e^{\hat{i}})^T Tx$. Hence, g is certainly costly to compute and we require an efficient rootfinder to speed the convergence of the limit point routine. A specially modified version of the routine given in [4] is used in our program. Clearly, as in the case of target points, we may fail to detect a limit point if the continuation steps are too large and in such a situation the rootfinder may also fail to converge. In addition, the evaluation of g may run into difficulties when the desired limit point is near a bifurcation point.

6. SOME NUMERICAL EXAMPLES

The programs described here have been used extensively with excellent success on problems from many different areas. We include here only a few numerical examples to illustrate the operation of the programs.

Example 1. In order to present some details of the performance of the programs we consider first a very small problem which was originally formulated in [9] and subsequently used as a test case by many authors. The mapping F has here the form

$$(6.1) \quad Fx = \begin{pmatrix} x_1 - x_2^3 + 5x_2^2 - 2x_2 + 34x_3 - 47 \\ x_1 + x_2^3 + x_2^2 - 14x_2 + 10x_3 - 39 \end{pmatrix}, \quad \forall x \in \mathbb{R}^3.$$

For the starting point $x^0 = (15, -2, 0)^T$ the solution curve passes through $x^* = (5, 4, 1)^T$ and this point is chosen as target.

Tables 2 and 3 show runs with the full Newton method and modified Newton method, respectively as corrector process. A starting step $h_0 = 0.3$ and maximum step $h_{\max} = 25.0$ were used. The performance for the two correctors is practically the same although the step-prediction exhibits certain differences due to our assessment of the corrector distance. Clearly, the use of the modified Newton process is much less expensive and hence preferable as Table 4 shows which summarizes the total number of function and Jacobian calls including those for the target calculation. Comparative performance data given in [7] for this problem involved 22 continuation steps, 15 step reductions and 128 Jacobian evaluations. The procedure discussed in [19] required 25 continuation steps but no further details were provided in the paper.

Step	Continuation point			Contin. Variable	Total Correct. Steps	Comments
	x_1	x_2	x_3			
0	15.000	-2.00000	0.00000	x_3	—	
1	14.705	-1.9421	0.065381	x_1	2	
2	14.285	-1.7291	0.26874	x_3	3	
3	16.906	-1.2094	0.54684	x_2	2	
4	24.918	-0.59908	0.55514	x_1	3	
5	48.974	0.71803	-0.080758	x_1	3	
6	57.928	1.2846	-0.40736	x_1	4	Step red.
7	60.052	1.5709	-0.54035	x_1	4	Step red.
8	61.666	2.0010	-0.66683	x_2	2	
9	-5.1039	4.1510	1.3464	x_2	2	Target passed
TOTAL					25	
Computation of target					4	

Table 2

Step	Continuation point			Contin. Variable	Total Correct Steps	Comments
	x_1	x_2	x_3			
0	15.000	-2.0000	0.00000	x_3	—	
1	14.710	-1.9421	0.065381	x_1	3	
2	14.285	-1.7291	0.26874	x_3	4	
3	16.906	-1.2094	0.54685	x_2	1	
4	24.918	-0.59906	0.55514	x_1	6	
5	48.975	0.71810	-0.080804	x_1	5	
6	57.289	1.2847	-0.40742	x_1	6	Step red.
7	60.053	1.5711	-0.54042	x_1	5	Step red.
8	61.666	2.0013	-0.66689	x_2	2	
9	-4.4239	4.1413	1.3229	x_2	1	Target passed
TOTAL					33	
Computation of target					8	

Table 3

	Corrector Process	
	Newton	Mod. Newton
Function calls	41	53
Jacobian calls	38	21

Table 4

It may be noted that the solution curve has two limit points each with respect to x_1 and x_3 . The two step reductions are almost unavoidable here since the curve has a long straight segment followed by a very sharp bend. The target computation is relatively expensive since the last step is extremely large due to another straight curve segment.

Example 2. Maneuvering airplanes, especially at high angles of attack, sometimes undergo sudden jumps in their response to the pilot's control inputs. The problem has been discussed extensively in the literature, see, for example, [18], [30], [39]. Without going into further details we use here a simplified version of a system of five equilibrium equations involving the roll rate (x_1), pitch rate (x_2), yaw rate (x_3), (incremental) angle of attack (x_4), side slip angle (x_5), elevator angle (x_6), aileron angle (x_7), and rudder angle (x_8). More specifically, for the particular aircraft discussed in [18] these equations have the dimensionless form

$$(6.1) \quad Fx \equiv Ax + \phi(x) = 0, \quad \forall x \in R^8$$

where

$$A = \begin{pmatrix} -3.933 & 0.107 & 0.126 & 0 & -9.99 & 0 & -45.83 & -7.64 \\ 0 & -0.987 & 0 & -22.95 & 0 & -28.37 & 0 & 0 \\ 0.002 & 0 & -0.235 & 0 & 5.67 & 0 & -0.921 & -6.51 \\ 1.0 & 0 & 0 & -1.0 & 0 & -0.168 & 0 & 0 \\ 0 & 0 & -1.0 & 0 & -0.196 & 0 & -0.0071 & 0 \end{pmatrix}$$

and

$$\phi(x) = \begin{pmatrix} -0.727 x_2 x_3 + 8.39 x_3 x_4 - 684.4 x_4 x_5 + 63.5 x_4 x_7 \\ 0.949 x_1 x_3 + 0.173 x_1 x_5 \\ -0.716 x_1 x_2 - 1.578 x_1 x_4 + 1.132 x_4 x_7 \\ -x_1 x_2 \\ x_1 x_4 \end{pmatrix}.$$

Figure 3 shows some solution curves on the three-dimensional equilibrium surface in R^8 . More specifically, in all cases we fixed a value of x_6 (elevator deflection) and chose the rudder deflection $x_8 = 0$. The paths $x_6 > \omega_1$, $x_8 = 0$ with $\omega_1 \approx -0.0061771$ have two limit points, for $\omega_1 > x_6 > \omega_2$, $x_8 = 0$, with $\omega_2 \approx -0.012498$ a third limit point appears, and for $\omega_2 > x_6$, $x_8 = 0$ only one limit point remains. A similar picture arises for negative roll rates.

In all cases the programs easily detected and computed the various limit points (see Table 5). But the example also shows that even with a large number of search paths it is difficult to provide a full picture of the location of the critical boundary, that is, of the curves of limit points with respect to x_1 for $x_8 = 0$ and varying x_6, x_7 . In Figure 3 the corresponding branches of limit point curves are shown as dotted lines. They were obtained with a code for the

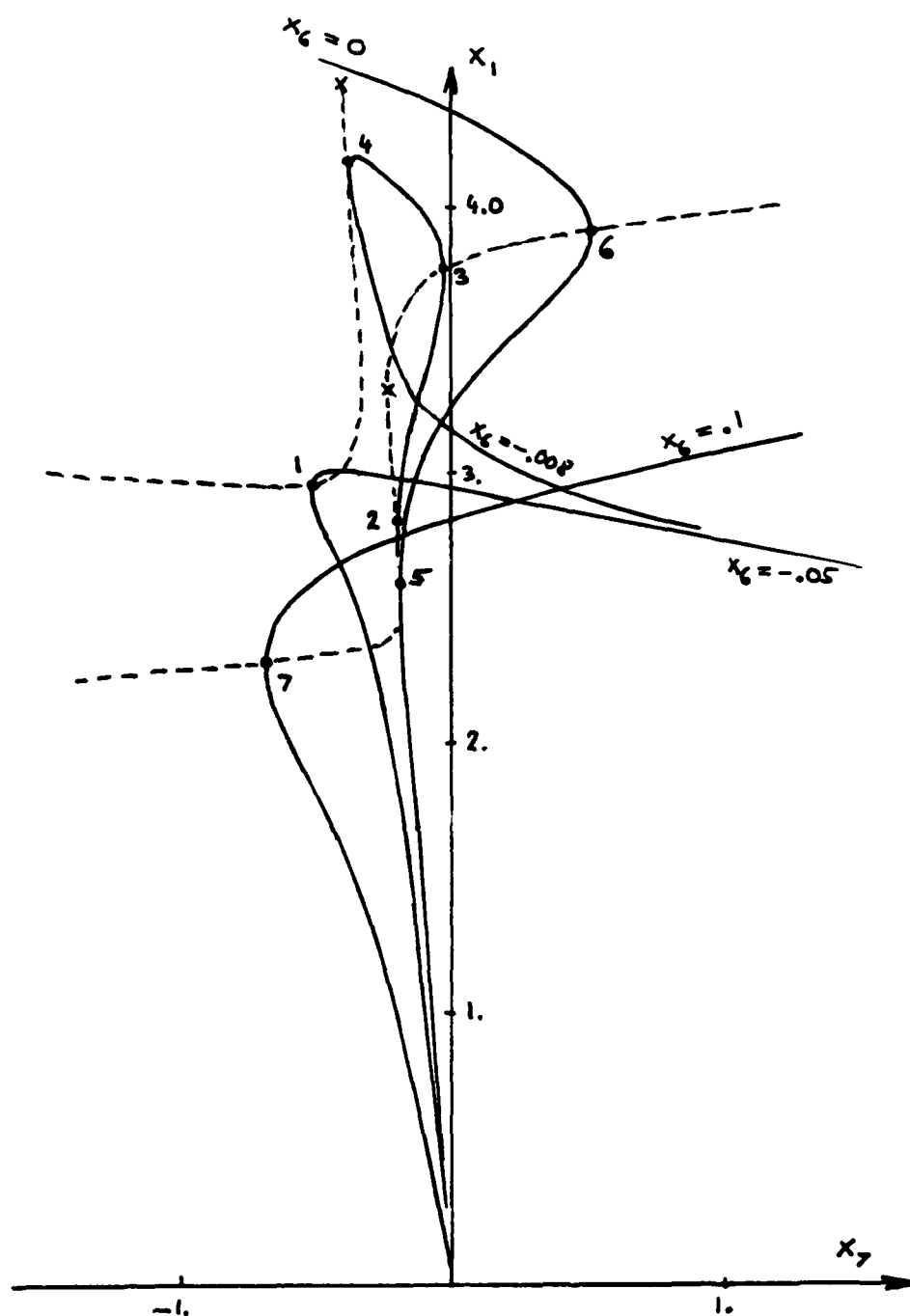


Figure 3

earlier mentioned task (1.3) (iv) (see [28]).

	x_1	x_2	x_3	x_4	x_5	x_6	x_7
1	2.9649	0.82557	0.073661	0.041309	0.26735	-0.05	0.50481
2	2.8174	-0.17629	0.089926	0.026429	-0.071476	-0.008	-0.20497
3	3.7579	-0.65542	0.38658	0.092521	-0.19867	-0.008	0.006208
4	4.1638	0.089131	0.094806	0.022889	0.016232	-0.008	-0.37766
5	2.5873	-0.22355	0.054682	0.013676	-0.091687	0.0	-0.18691
6	3.9005	-1.1482	0.58156	0.13352	-0.32859	0.0	0.51016
7	2.2992	-1.4102	-0.061849	-0.079009	-0.58630	0.1	-0.68972
8	4.4565	-4.4909	1.6164	0.33091	-1.0857	0.1	10.0212

Table 5

Example 3. As an example for the numerical investigation of the equilibrium surface of a mechanical structure, we consider a clamped, thin, shallow, circular arch which has been used as a test case by various authors (see eg. [12], [16], [36]). Let U and W be the radial and axial displacements, R the arch radius, A the cross-sectional area, H the thickness, and E Young's modulus. With the dimensional displacements $u = U/H$, $w = W/H$, the total potential energy -- non-dimensionalized by dividing by $EAR(H/R)^2$ --

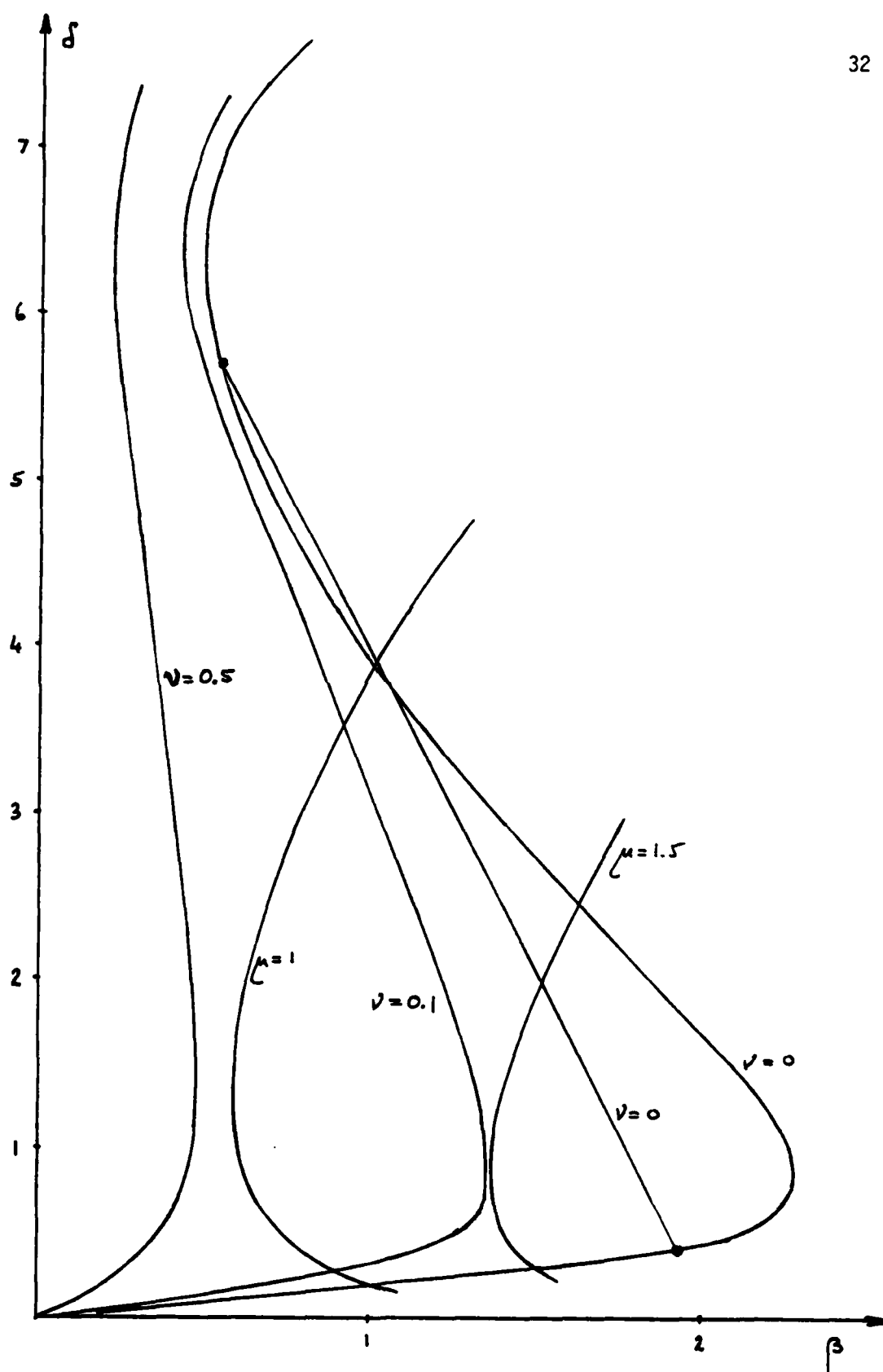


Figure 4

is given by

$$(6.2) \quad \int_{-\theta_0}^{\theta_0} \left\{ \left[\left(\frac{dw}{d\theta} - u \right) + \frac{1}{2} \frac{H}{R} \left(\frac{du}{d\theta} \right)^2 \right]^2 + \alpha_1 \left(\frac{d^2 u}{d\theta^2} \right)^2 - \alpha_2 p u \right\} d\theta.$$

Here $p = p(\theta)$ is the dimensionless radial load, and α_1, α_2 are dimensionless constants. Each end is assumed to be pinned, that is, we have the boundary conditions

$$(6.3) \quad u(\pm \theta_0) = 0, \quad w(\pm \theta_0) = 0, \quad \frac{d^2 u}{d\theta^2}(\pm \theta_0) = 0.$$

The finite element approximation introduced in [36] was applied. More specifically, we used a uniform mesh with eight elements, $\theta_0 = 15$ and the constants $\alpha_1 = 3.8716 \times 10^{-6}$, $\alpha_2 = 1.65504 \times 10^{-1}$ corresponding to the data in [16]. Moreover, the following load function $p = p(\mu, \nu)$ was chosen

$$(6.4) \quad p(\mu, \nu) = \begin{cases} \mu(1 + 7\nu), & \text{for element 4} \\ \mu(1 - \nu), & \text{otherwise} \end{cases}$$

corresponding to a base load $\beta = \mu(1 - \nu)$ and an excess load $8\mu\nu$ in element 4 such that the average load is always μ .

Several curves on the equilibrium surface corresponding to constant values of μ or ν were computed. Figure 4 shows the projection of these curves into the (β, δ) -plane where δ represents the radial displacement of the center point. For uniform loads, that is, $\nu = 0$, we encounter two bifurcation points on the primary curve which are connected by two "buckling" curves that have the same projection in the (β, δ) -plane.

7. THE PITCON CODE

```

SUBROUTINE PITCON(NVAR,I M,IT,XIT,KSTEP,IPC,H,TRET,IMOD,IPVT,
1 HMAX,HMIN,HFACT,ABSERR,ERR,WORK,ISIZE)
C*****
C
C PITCON.FOR
C
C 29 OCT 1981 VERSION OF PITCON,
C THE UNIVERSITY OF PITTSBURGH CONTINUATION PACKAGE.
C THIS VERSION USES SINGLE PRECISION AND FULL MATRIX STORAGE.
C
C THIS PACKAGE WAS PREPARED WITH THE PARTIAL SUPPORT OF
C THE NATIONAL SCIENCE FOUNDATION, UNDER GRANT MCS-78-05299,
C
C BY WERNER C. RHEINBOLDT AND JOHN V. BURKARDT
C INSTITUTE FOR COMPUTATIONAL MATHEMATICS AND APPLICATIONS
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C
C AN EARLIER VERSION OF THE PACKAGE WAS WRITTEN IN COOPERATION WITH
C GEORGE D BYRNE,
C COMPUTING TECHNOLOGY AND SERVICES
C EXXON RESEARCH AND ENGINEERING COMPANY
C LINDEN, NEW JERSEY, 07036
C
C THIS PACKAGE COMPUTES POINTS ALONG A SOLUTION CURVE OF AN
C UNDERDETERMINED SYSTEM OF NONLINEAR EQUATIONS OF THE FORM  $FX=0$ .
C THE CURVE IS SPECIFIED TO PASS THROUGH A GIVEN STARTING SOLUTION
C  $X$  OF THE SYSTEM. HERE  $X$  DENOTES A REAL VECTOR OF NVAR
C COMPONENTS AND  $FX$  A REAL VECTOR OF NVAR-1 COMPONENTS.
C NORMALLY EACH CALL TO PITCON PRODUCES A NEW POINT FURTHER ALONG
C THE SOLUTION CURVE IN A USER-SPECIFIED DIRECTION.
C AN OPTION ALLOWS THE SEARCH FOR AND COMPUTATION OF TARGET POINTS,
C THAT IS, SOLUTION POINTS  $X$  FOR WHICH  $X(IT) = XIT$  FOR SOME USER
C SPECIFIED VALUES OF  $IT$  AND  $XIT$ .
C A FURTHER OPTION ALLOWS THE SEARCH FOR AND COMPUTATION OF LIMIT
C POINTS FOR SPECIFIED COORDINATE  $LIM$ , THAT IS, SOLUTION POINTS FOR
C WHICH THE  $LIM$ -TH COMPONENT OF THE TANGENT VECTOR IS ZERO.
C
C EXPLANATIONS OF THE ALGORITHMS USED IN THIS PACKAGE MAY
C BE FOUND IN THE FOLLOWING REFERENCES:
C
C WERNER RHEINBOLDT,
C SOLUTION FIELD OF NONLINEAR EQUATIONS AND CONTINUATION METHODS
C SIAM JOURNAL OF NUMERICAL ANALYSIS, 17, 1980, PP 221-237
C
C COR DEN HEIJER AND WERNER RHEINBOLDT,
C ON STEPLENGTH ALGORITHMS FOR A CLASS OF CONTINUATION METHODS,
C SIAM JOURNAL OF NUMERICAL ANALYSIS 18, 1981, PP 925-947
C
C WERNER RHEINBOLDT,
C NUMERICAL ANALYSIS OF CONTINUATION METHODS FOR NONLINEAR
C STRUCTURAL PROBLEMS,
C COMPUTERS AND STRUCTURES, 13, 1981, PP 103-114
C
C OUTLINE OF THE MATHEMATICAL PROCEDURE
C
C THE FUNCTION  $F$  DEFINING THE SYSTEM OF EQUATIONS IS SUPPOSED TO
C BE CONTINUOUSLY DIFFERENTIABLE. THE REGULARITY SET  $R(F)$  OF  $F$  IS
C THE SET OF ALL POINTS  $X$  IN NVAR-DIMENSIONAL SPACE WHERE THE
C DERIVATIVE  $DF(X)$  HAS MAXIMAL RANK. THE STARTING POINT IS ASSUMED
C TO BE IN  $R(F)$ . FOR ANY INDEX  $IP$  WITH  $1 \leq IP \leq NVAR$ , LET

```

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 PTCN0003
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 PTCN0062
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 PTCN0065
 PTCN0066
 PTCN0067
 PTCN0068
 PTCN0069
 PTCN0070

C FA(X,IP) BE THE FUNCTION OBTAINED BY AUGMENTING F WITH
 C AN NVAR-TH SCALAR FUNCTION X(IP)-R FOR SOME NUMMER R. FOR ANY
 C X IN R(F) THERE IS AT LEAST ONE INDEX IP SUCH THAT THE DERIVATIVE
 C DFA(X,IP) OF FA IS NONSINGULAR. WITH SUCH AN IP, AND A DIRECTION
 C DIR (=+1 OR -1), THE TANGENT OF FA, TAN(X), IS UNIQUELY DEFINED BY:
 C
 C TAN:= SOLUTION OF (DFA(X,IP)*TAN=E(NVAR))
 C TAN:= TAN/(EUCLIDEAN NORM OF TAN)
 C SN:= DIR*SIGN (DETERMINANT (DFA(X,IP)))
 C TAN:= SN*TAN

C HERE E(I) IS THE I-TH BASIS VECTOR IN NVAR-SPACE.
 C THE PROCESS USES A LOCAL PARAMETERIZATION OF THE CURVE.
 C NORMALLY THE CONTINUATION PARAMETER INDEX IP IS CHOSEN AS
 C THAT INDEX FOR WHICH ABS(TAN(X)(IP)) IS MAXIMAL. BUT IN THE
 C CASE OF CERTAIN CURVATURE CHANGES WHERE IT APPEARS THAT
 C A LIMIT POINT FOR THIS CHOICE FOR IP IS APPROACHING,
 C OTHER CHOICES FOR IP MAY BE USED.

C PREDICTION TAKES PLACE ALONG THE EULER LINE X+H*TAN. THE
 C STEPLENGTH ALGORITHM TAKES INTO ACCOUNT THE QUALITY OF THE
 C CORRECTOR ITERATION AT THE LAST POINT AND A PREDICTION OF THE
 C CHANGE IN CURVATURE. THE TANGENTIAL STEPSIZE USED IN PREDICTION IS
 C CHOSEN SO AS TO ACHIEVE APPROXIMATELY THE PREDICTED SECANT STEPSIZE
 C AFTER CORRECTION IS DONE.

C THE CORRECTOR ITERATION STARTS FROM THE PREDICTED POINT AND SOLVES
 C THE AUGMENTED SYSTEM FA(X,IP)=0 WITH THE VALUE OF THE SCALAR
 C B EQUAL TO THE IP-TH COMPONENT OF THE PREDICTED POINT. THE USER
 C CAN SPECIFY AS CORRECTOR ITERATION EITHER A FULL NEWTON PROCESS,
 C OR A MODIFIED NEWTON PROCESS WITH FIXED JACOBIAN DFA EVALUATED AT
 C THE PREDICTED POINT.

C OUTLINE OF THE COMPUTATIONAL ALGORITHM

C DURING THE FOLLOWING DESCRIPTION, WE WILL ASSUME THAT WE
 C HAVE ENTERED THE CONTINUATION LOOP WITH AN OLD POINT XL,
 C A CURRENT POINT XC, THE TANGENT TL AT XL, AND CERTAIN SCALAR
 C QUANTITIES ASSOCIATED WITH THESE VECTORS. WE WILL CHECK
 C FIRST FOR ANY TARGET OR LIMIT POINTS BETWEEN XL AND XC,
 C THEN PROCEED TO COMPUTE A NEW CONTINUATION POINT XF.
 C THESE NAMES ARE NOT IN PRECISE ACCORDANCE WITH THE STORAGE
 C ARRANGEMENTS UNTIL THE END OF A CONTINUATION STEP.

C STEP 1: FOR KSTEP.GT.0, THE CODE GOES TO STEP 2.
 C ON THE FIRST CALL TO PITCON FOR A GIVEN PROBLEM (KSTEP=-1
 C OR KSTEP=0) PROBLEM-DEPENDENT CONSTANTS ARE SET
 C AND USER CONTROL PARAMETERS ARE LOADED OR DEFAULTS USED.
 C IF (KSTEP.EQ.0), THE PROGRAM PROCEEDS TO STEP 2.
 C IF (KSTEP.EQ.-1), THE USER REQUESTS THAT THE INPUT STARTING
 C POINT XR BE CHECKED FOR THE CONDITION
 C ABS(F(XR)).LE.(ABSERR/2). IF THIS IS NOT THE CASE, NEWTON'S
 C METHOD IS APPLIED TO THE POINT XR UNTIL THE ERROR CONDITION
 C IS SATISFIED, OR A FAILURE HAS OCCURRED. AN UNIMPROVABLE
 C POINT RESULTS IN A RETURN OF IRET=-6.
 C IF THE STARTING POINT XR WAS IMPROVED, THE PROGRAM RETURNS
 C WITH IRET=0 AND KSTEP=0.
 C IF (KSTEP.EQ.0), THE CONTINUATION LOOP BEGINS WITH THE
 C STARTING POINT XR STORED IN XL AND XC, THE STEPSIZE HTANCE
 C SET TO THE INPUT VALUE OF H, AND THE
 C CONTINUATION PARAMETER SET TO THE INPUT VALUE OF IPC.
 C FOR KSTEP.GT.0, THESE QUANTITIES ARE COMPUTED AND
 C UPDATED BY THE PROGRAM ITSELF.

C STEP 2: TARGET POINT CHECK. IF (IT.NE.0), A TARGET POINT IS
 C DESIRED. THE VALUES OF XL(IT) AND XC(IT) ARE COMPARED TO
 C XIT. IF THE TARGET POINT IS BETWEEN XL AND XC, THE PROGRAM
 C COMPUTES THE TARGET POINT, SETS IRET=1, AND
 C RETURNS, TEMPORARILY INTERRUPTING NORMAL CONTINUATION.

PTCN0071
 PTCN0072
 PTCN0073
 PTCN0074
 PTCN0075
 PTCN0076
 PTCN0077
 PTCN0078
 PTCN0079
 PTCN0080
 PTCN0081
 PTCN0082
 PTCN0083
 PTCN0084
 PTCN0085
 PTCN0086
 PTCN0087
 PTCN0088
 PTCN0089
 PTCN0090
 PTCN0091
 PTCN0092
 PTCN0093
 PTCN0094
 PTCN0095
 PTCN0096
 PTCN0097
 PTCN0098
 PTCN0099
 PTCN0100
 PTCN0101
 PTCN0102
 PTCN0103
 PTCN0104
 PTCN0105
 PTCN0106
 PTCN0107
 PTCN0108
 PTCN0109
 PTCN0110
 PTCN0111
 PTCN0112
 PTCN0113
 PTCN0114
 PTCN0115
 PTCN0116
 PTCN0117
 PTCN0118
 PTCN0119
 PTCN0120
 PTCN0121
 PTCN0122
 PTCN0123
 PTCN0124
 PTCN0125
 PTCN0126
 PTCN0127
 PTCN0128
 PTCN0129
 PTCN0130
 PTCN0131
 PTCN0132
 PTCN0133
 PTCN0134
 PTCN0135
 PTCN0136
 PTCN0137
 PTCN0138
 PTCN0139
 PTCN0140

C STEP 3: TANGENT AND LOCAL CONTINUATION PARAMETER CALCULATION. IF THE
 C LOOP WAS SUSPENDED AT THE LAST CALL TO FITCON TO ALLOW THE
 C RETURN OF A LIMIT POINT, THEN THE TANGENT HAS ALREADY BEEN
 C CALCULATED AND A LIMIT POINT CHECK IS SUPERFLUOUS, SO
 C THE PROGRAM SKIPS TO STEP 5.
 C OTHERWISE, A VECTOR IN THE TANGENT PLANE AT XC IS COMPUTED.
 C SUPPOSE THAT THE PREVIOUS CONTINUATION PARAMETER INDEX
 C WAS IPL, WHERE ON THE FIRST STEP IPL IS USER-SUPPLIED.
 C THE NEW TANGENT IS NORMALIZED, AND THE IPL-TH COMPONENT
 C IS FORCED TO HAVE THE SAME SIGN AS THE IPL-TH COMPONENT
 C OF THE PREVIOUS TANGENT (OR ON FIRST STEP, THE SAME
 C SIGN AS THE USER INPUT DIRECTION DIR.) THEN THE LOCAL
 C CONTINUATION PARAMETER IPC IS DETERMINED. IPC IS SET TO THE
 C LOCATION OF THE LARGEST COMPONENT OF THE TANGENT VECTOR
 C UNLESS A LIMIT POINT FOR THIS CHOICE APPEARS TO BE
 C APPROACHING, IN WHICH CASE THE LOCATION OF THE SECOND
 C LARGEST COMPONENT MAY BE TRIED.
 C ONCE IPC IS SET, THE QUANTITIES TCIPC, TCLIM, HSFCLC, ALPHLC
 C AND DIR ARE COMPUTED, WHOSE MEANINGS ARE EXPLAINED BELOW.
 C
 C STEP 4: LIMIT POINT CHECK. IF LIM.NE.0, THE LIM-TH COMPONENTS
 C OF THE OLD AND NEW TANGENTS ARE COMPARED. IF THESE DIFFER
 C IN SIGN, A LIMIT POINT LIES BETWEEN XL AND XC. THE PROGRAM
 C ATTEMPTS TO FIND THIS LIMIT POINT. IF FOUND, IT STORES
 C THE LIMIT POINT IN XR, THE TANGENT AT XR IN TL, SETS IRET=2,
 C AND RETURNS, TEMPORARILY INTERRUPTING THE NORMAL LOOP.
 C
 C STEP 5: STEP LENGTH COMPUTATION. THE PROGRAM COMPUTES HTANCF, THE
 C STEPSIZE TO BE USED ALONG THE TANGENT TO OBTAIN THE
 C PREDICTED POINT XPRED:=XC+HTANCF*TC, THE STARTING POINT
 C FOR THE CORRECTOR PROCESS. IN COMPUTING HTANCF, CERTAIN
 C CURVATURE AND STEPSIZE DATA ARE UPDATED.
 C
 C STEP 6: PREDICTION AND CORRECTION STEP. WITH THE PREDICTED POINT
 C XPRED=XC+HTANCF*TC AS A STARTING POINT, THE CORRECTOR
 C PROCESS IS APPLIED TO CORRECT THE POINT UNTIL
 C ABS(F(XCOR)).LE.ABSERR AND XSTEP, THE LAST CORRECTOR STEP,
 C SATISFIES XSTEP.LE.ABSERR+RELERR*ABS(XCOR).
 C IF THE SIZE OF A CORRECTOR STEP IS TOO LARGE,
 C OR IF A CORRECTION STEP INCREASES THE FUNCTION VALUE, OR
 C THE MAXIMUM NUMBER OF STEPS ARE TAKEN WITHOUT CONVERGENCE,
 C THE STEPSIZE HTANCF IS REDUCED AND THE CORRECTOR STEP IS
 C ATTEMPTED AGAIN. IF THE STEPSIZE SHRINKS BELOW HMIN, THE
 C PROGRAM SETS AN ERROR FLAG AND RETURNS.
 C
 C STEP 7: STORING INFORMATION BEFORE RETURN. AFTER A SUCCESSFUL
 C CONTINUATION STEP, THE PROGRAM REARRANGES ITS STORAGE SO
 C THAT THE ENTRIES CORRESPONDING TO XC AND XF HOLD THE PROPER
 C DATA, COMPUTES CORDIS, THE SIZE OF THE CORRECTION TO THE
 C PREDICTED POINT, AND MODIFIES CORDIS TO A VALUE THAT WOULD
 C CORRESPOND TO AN OPTIMAL NUMBER OF CORRECTOR STEPS.
 C
 C ON NORMAL RETURN, THE VECTOR XR (THE FIRST NVAR ENTRIES OF RWORK),
 C CONTAINS A SOLUTION POINT ON THE CURVE F(XR)=0, AND IS EITHER
 C A CONTINUATION POINT, A TARGET POINT, OR A LIMIT POINT, WHICH
 C IS INDICATED BY THE VALUE OF IRET.
 C IF IRET IS NEGATIVE, AN ERROR HAS OCCURRED. IF A LIMIT POINT IS
 C RETURNED, THE TANGENT VECTOR AT THE LIMIT POINT IS CONTAINED IN THE
 C LOCATION TL IN RWORK. ON FIRST CALL, THE USER MUST SET SOME OF THE
 C SCALAR PARAMETERS, AND THE STARTING POINT XR. THEREAFTER, ONLY IT
 C AND XJT SHOULD BE CHANGED BY THE USER DURING A PROBLEM RUN.
 C IF A NEW PROBLEM IS TO BE RUN (WHETHER A DIFFERENT FUNCTION, OR THE
 C SAME FUNCTION WITH DIFFERENT STARTING POINT OR ERROR CONTROLS)
 C THE PROGRAM MAY BE RESET BY USING KSTEP=-1 OR 0, AT WHICH TIME THE
 C SCALARS AND THE POINT XR MUST BE SET AGAIN. NOTE THAT IN THIS CASE
 C THE STATISTICAL DATA IN THE COMMON BLOCKS /COUNT1/ AND /COUNT2/
 C WILL BE RESET TO 0 AS WELL.

PTCN0141
 PTCN0142
 PTCN0143
 PTCN0144
 PTCN0145
 PTCN0146
 PTCN0147
 PTCN0148
 PTCN0149
 PTCN0150
 PTCN0151
 PTCN0152
 PTCN0153
 PTCN0154
 PTCN0155
 PTCN0156
 PTCN0157
 PTCN0158
 PTCN0159
 PTCN0160
 PTCN0161
 PTCN0162
 PTCN0163
 PTCN0164
 PTCN0165
 PTCN0166
 PTCN0167
 PTCN0168
 PTCN0169
 PTCN0170
 PTCN0171
 PTCN0172
 PTCN0173
 PTCN0174
 PTCN0175
 PTCN0176
 PTCN0177
 PTCN0178
 PTCN0179
 PTCN0180
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 PTCN0182
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 PTCN0186
 PTCN0187
 PTCN0188
 PTCN0189
 PTCN0190
 PTCN0191
 PTCN0192
 PTCN0193
 PTCN0194
 PTCN0195
 PTCN0196
 PTCN0197
 PTCN0198
 PTCN0199
 PTCN0200
 PTCN0201
 PTCN0202
 PTCN0203
 PTCN0204
 PTCN0205
 PTCN0206
 PTCN0207
 PTCN0208
 PTCN0209
 PTCN0210

DEFINITIONS AND DEFAULTS OF PITCON PARAMETERS

NVAR = THE NUMBER OF VARIABLES IN THE NONLINEAR SYSTEM. NVAR IS THE DIMENSION OF THE PIVOT VECTOR IPVT, AND THE SIZE OF THE VECTORS XR, XC, XF, TL AND TC WHICH ARE CONTAINED IN RWORK. RWORK ALSO CONTAINS STORAGE FOR THE MATRIX FPRYM WHICH IS OF SIZE NVAR X NVAR. NVAR MUST BE GREATER THAN 1, AND MUST NOT BE CHANGED DURING THE COURSE OF A PROBLEM RUN. NVAR HAS NO DEFAULT VALUE.

LIM = LIMIT POINT FLAG AND INDEX. IF (LIM.EQ.0), LIMIT POINTS ARE NOT TO BE LOOKED FOR. OTHERWISE, THE USER SHOULD SET LIM TO THE INDEX OF THE VARIABLE FOR WHICH LIMIT POINTS ARE TO BE SOUGHT. LIM DEFAULTS TO ZERO. LIM MUST SATISFY 0.LE.LIM.LE.NVAR.

IT = TARGET POINT FLAG AND INDEX. IF (IT.EQ.0), TARGET POINTS ARE NOT TO BE LOOKED FOR. OTHERWISE, THE USER SHOULD SET IT TO THE INDEX OF THE VARIABLE FOR WHICH TARGET VALUES XIT ARE DESIRED. IT HAS THE DEFAULT VALUE ZERO. IT MAY BE RESET BY THE USER AT ANY TIME DURING A RUN. IT MUST SATISFY 0.LE.IT.LE.NVAR.

XIT = THE VALUE OF THE TARGET VECTOR COMPONENT SOUGHT, IF IT.NE.0. TARGET POINTS XR SATISFY XR(IT)=XIT. XIT HAS NO DEFAULT.

KSTEP = THE NUMBER OF CONTINUATION STEPS TAKEN. THIS DOES NOT INCLUDE FAILURES, TARGET POINTS OR LIMIT POINTS. THE PROGRAM INCREMENTS KSTEP EACH TIME A NEW POINT XF IS COMPUTED. ON THE FIRST CALL TO PITCON FOR A PARTICULAR PROBLEM, THE USER SHOULD SET KSTEP TO 0 OR -1. IF KSTEP=-1, THE PROGRAM WILL CHECK THE ACCURACY OF THE STARTING POINT XR, AND IF NECESSARY, ATTEMPT TO CORRECT IT USING NEWTON'S METHOD. IF KSTEP=0, THE PROGRAM PERFORMS NO CHECK ON THE STARTING POINT, AND PROCEEDS TO THE CONTINUATION LOOP. IF THE USER WISHES TO RUN A DIFFERENT PROBLEM THEN A CALL TO PITCON WITH KSTEP=-1 OR 0 WILL RESET THE CODE, DESTROYING THE INFORMATION FROM THE PREVIOUS RUN. KSTEP DEFAULTS TO -1.

IPC = THE COMPONENT OF XC TO BE USED AS CONTINUATION PARAMETER. ON THE FIRST CALL ONLY, THE USER OUGHT TO SET IPC OR ALLOW THE DEFAULT VALUE IPC=NVAR. AFTER THE FIRST CALL, THE DETERMINATION OF IPC IS DONE BY THE PROGRAM USING INFORMATION ABOUT THE TANGENT VECTOR AT XC.

H = SUGGESTED STARTING STEP SIZE ALONG THE TANGENT TO THE CURVE. IF H=0.0 ON THE INITIAL CALL, H DEFAULTS TO (HMAX+HMIN)/2. IF H IS NEGATIVE ON THE FIRST CALL, THE MINUS SIGN IS ABSORBED BY DIR AND INDICATES THAT THE DIRECTION OF THE FIRST STEP SHOULD BE IN THE NEGATIVE IPC DIRECTION. AFTER THE FIRST STEP, STEPSIZE IS CONTROLLED BY THE PROGRAM. UPON RETURN WITH A CONTINUATION POINT (IRET=0), H IS OVERWRITTEN BY HTANCF, THE STEPSIZE USED IN REACHING THE NEW POINT.

IRET = A RETURN FLAG TO INDICATE ERRORS OR THE TYPE OF POINT RETURNED IN XR. NONNEGATIVE VALUES OF IRET REPRESENT NORMAL RETURNS. NEGATIVE VALUES OF IRET INDICATE THAT SOME ERROR OR DIFFICULTY HAS BEEN ENCOUNTERED. VALUES OF IRET BETWEEN -1 AND -4 ARE SIMPLY REPORTS THAT AN ATTEMPT TO COMPUTE A LIMIT OR TARGET POINT FAILED. THESE DO NOT AFFECT FURTHER CONTINUATION STEPS, AND THE USER NEED NOT MODIFY ANY VARIABLES BEFORE PROCEEDING. VALUES OF IRET OF -5 AND -6 REFER TO DANGEROUS SITUATIONS THAT MAY BE CORRECTABLE. VALUES OF IRET FROM -7 TO -10 ARE SERIOUS, FATAL ERRORS. THE USER SHOULD HALT THE PROGRAM AND EXAMINE HIS INPUT AND THE INTERIM RESULTS. IRET SHOULD BE ZERO ON THE FIRST CALL FOR A PROBLEM. THE SPECIFIC VALUES OF IRET AND THEIR MEANINGS ARE:

IRET=2: NORMAL RETURN WITH LIMIT POINT IN XR AND TANGENT AT XR CONTAINED IN TL.

IRET=1: NORMAL RETURN WITH TARGET POINT IN XR.

PTCN0211
PTCN0212
PTCN0213
PTCN0214
PTCN0215
PTCN0216
PTCN0217
PTCN0218
PTCN0219
PTCN0220
PTCN0221
PTCN0222
PTCN0223
PTCN0224
PTCN0225
PTCN0226
PTCN0227
PTCN0228
PTCN0229
PTCN0230
PTCN0231
PTCN0232
PTCN0233
PTCN0234
PTCN0235
PTCN0236
PTCN0237
PTCN0238
PTCN0239
PTCN0240
PTCN0241
PTCN0242
PTCN0243
PTCN0244
PTCN0245
PTCN0246
PTCN0247
PTCN0248
PTCN0249
PTCN0250
PTCN0251
PTCN0252
PTCN0253
PTCN0254
PTCN0255
PTCN0256
PTCN0257
PTCN0258
PTCN0259
PTCN0260
PTCN0261
PTCN0262
PTCN0263
PTCN0264
PTCN0265
PTCN0266
PTCN0267
PTCN0268
PTCN0269
PTCN0270
PTCN0271
PTCN0272
PTCN0273
PTCN0274
PTCN0275
PTCN0276
PTCN0277
PTCN0278
PTCN0279
PTCN0280

IRET=0: NORMAL RETURN WITH NEW CONTINUATION POINT IN XR. PTCN0281
 IRET=-1: AN ERROR OCCURRED DURING COMPUTATION OF LIMIT POINT PTCN0282
 IRET=-2: CORECT CALLED FOR TARGET POINT CALCULATION FAILED PTCN0283
 AFTER KNMAX ITERATIONS. PTCN0284
 IRET=-3: SOLVE WAS CALLED BY CORECT FOR TARGET POINT PTCN0285
 CALCULATION, AND FAILED. (MATRIX ELIMINATION FOUND PTCN0286
 ZERO PIVOT). PTCN0287
 IRET=-4: UNACCEPTABLE CORRECTOR STEP IN TARGET POINT PTCN0288
 CALCULATION. PTCN0289
 IRET=-5: PREDICTION STEP HTANCF IS LESS THAN HMIN, PERHAPS PTCN0290
 BECAUSE OF REPEATED FAILURE OF CORECT, AND PTCN0291
 CONSEQUENT STEPSIZE REDUCTION. USER MIGHT REDUCE PTCN0292
 HMIN, OR SWITCH FROM IMOD=1 TO IMOD=0, OR INCREASE PTCN0293
 ABSERR AND RELERR. BUT BE AWARE THAT REPEATED PTCN0294
 STEPSIZE REDUCTIONS MAY INDICATE AN INTRACTABLE PTCN0295
 FUNCTION. PTCN0296
 IRET=-6: FUNCTION VALUE FNRMXF OF INPUT XR IS TOO LARGE PTCN0297
 AND COULD NOT BE IMPROVED BY CORECT. USER PTCN0298
 MIGHT RECOVER BY RELAXING ERROR CONTROLS, IMPROVING PTCN0299
 STARTING POINT XR, OR CHANGING VALUE OF IPC. PTCN0300
 IRET=-7: SOLVE FAILED IN A CALL FROM TANGNT. PTCN0301
 IRET=-8: SOLVE FAILED IN A CALL FROM CORECT. PTCN0302
 IRET=-9: THE TANGENT VECTOR TC AT XC IS ZERO. PTCN0303
 IRET=-10: IMPROPER INPUT, NVAR.LE.1, OR PTCN0304
 ISIZE.LT.(NVAR)*(NVAR+5), OR PTCN0305
 PROGRAM HAS BEEN CALLED AGAIN AFTER FATAL ERROR. PTCN0306
 IMOD = METHOD FLAG FOR CORRECTOR STEP, SPECIFYING TYPE OF PTCN0307
 NEWTON METHOD TO BE USED. PTCN0308
 IMOD=0: UPDATE JACOBIAN FOR TANGENT CALCULATION, PTCN0309
 UPDATE JACOBIAN FOR EACH CORRECTOR STEP. PTCN0310
 IMOD=1: UPDATE JACOBIAN FOR TANGENT CALCULATION, PTCN0311
 EVALUATE JACOBIAN AT FIRST CORRECTOR STEP ONLY. PTCN0312
 IPVT = INTEGER VECTOR USER DECLARED TO BE OF SIZE NVAR. PTCN0313
 USED DURING THE MATRIX FACTORIZATION TO STORE PIVOT PTCN0314
 INFORMATION. PTCN0315
 HMAX = THE MAXIMUM STEP SIZE. IF HMAX.LE.0.0 ON INITIAL CALL, PTCN0316
 HMAX DEFAULTS TO SQRT(NVAR). PTCN0317
 HMIN = THE MINIMUM STEP SIZE. IF HMIN.LE.SQRT(EPMACH) ON INITIAL PTCN0318
 CALL, HMIN DEFAULTS TO SQRT(EPMACH), WHERE EPMACH IS THE PTCN0319
 MACHINE PRECISION CONSTANT. PTCN0320
 HFACT = LIMIT ON STEPSIZE CHANGE. HSECLC IS THE SECANT STEPSIZE PTCN0321
 OF THE LAST STEP, AND HTANCF IS THE STEPSIZE TO BE USED PTCN0322
 IN OBTAINING THE PREDICTED POINT. THE FOLLOWING RELATIONSHIP PTCN0323
 MUST BE SATISFIED: (HSECLC/HFACT).LE.HTANCF.LE.(HSECLC*HFACT) PTCN0324
 IF THE CORRECTOR STEP FAILS, THEN HFACT IS ALSO USED TO PTCN0325
 REDUCE THE PREDICTOR STEP HTANCF TO (HTANCF/HFACT) PTCN0326
 IF HFACT.LE.1.0 ON INITIAL CALL, HFACT DEFAULTS TO 3.0. PTCN0327
 ABSERR= ABSOLUTE ERROR CONTROL. IF ABSERR=0.0 ON INITIAL CALL PTCN0328
 ABSERR DEFAULTS TO SQRT(EPMACH) PTCN0329
 RELERR= RELATIVE ERROR CONTROL. IF RELERR=0.0 ON INITIAL CALL PTCN0330
 RELERR DEFAULTS TO SQRT(EPMACH) PTCN0331
 RWORK = USER DECLARED VECTOR OF SIZE ISIZE=NVAR*(NVAR+5). PTCN0332
 RWORK STORES FIVE VECTORS AND AN ARRAY IN THE ORDER PTCN0333
 (XR,XC,XF,TL,TC,FPRYM). THEIR BEGINNING LOCATIONS PTCN0334
 ARE IXR=1, IXC=NVAR+1, IXF=2*NVAR+1, ITL=3*NVAR+1. PTCN0335
 ITC=4*NVAR+1, IFP=5*NVAR+1. FPRYM IS AN ARRAY OF PTCN0336
 PTCN0337
 PTCN0338
 PTCN0339
 PTCN0340
 PTCN0341
 PTCN0342
 PTCN0343
 PTCN0344
 PTCN0345
 PTCN0346
 PTCN0347
 PTCN0348
 PTCN0349
 PTCN0350
 PTCN0351

SIZE NVAR X NVAR. THE MEANINGS OF THESE COMPONENTS OF RWORK ARE DESCRIBED BELOW. THE USER SHOULD SET A VALUE TO XRPTCN0352
ON FIRST CALL, BUT NO OTHER PORTIONS OF RWORK SHOULD BE SET. AFTER THE FIRST CALL FOR A PROBLEM, NO ENTRIES OF RWORK PTCN0353
SHOULD BE ALTERED. PTCN0354
PTCN0355
PTCN0356
PTCN0357
PTCN0358
PTCN0359
PTCN0360
PTCN0361
PTCN0362
PTCN0363
PTCN0364
PTCN0365
PTCN0366
PTCN0367
PTCN0368
PTCN0369
PTCN0370
PTCN0371
PTCN0372
PTCN0373
PTCN0374
PTCN0375
PTCN0376
PTCN0377
PTCN0378
PTCN0379
PTCN0380
PTCN0381
PTCN0382
PTCN0383
PTCN0384
PTCN0385
PTCN0386
PTCN0387
PTCN0388
PTCN0389
PTCN0390
PTCN0391
PTCN0392
PTCN0393
PTCN0394
PTCN0395
PTCN0396
PTCN0397
PTCN0398
PTCN0399
PTCN0400
PTCN0401
PTCN0402
PTCN0403
PTCN0404
PTCN0405
PTCN0406
PTCN0407
PTCN0408
PTCN0409
PTCN0410
PTCN0411
PTCN0412
PTCN0413
PTCN0414
PTCN0415
PTCN0416
PTCN0417
PTCN0418
PTCN0419
PTCN0420

(XR) = ON FIRST CALL, A USER SUPPLIED STARTING POINT, WHICH MAY BE IMPROVED BY THE PROGRAM IF KSTEP=-1. ON NORMAL RETURN FROM PITCON, XR WILL HOLD THE MOST RECENTLY FOUND POINT, WHETHER A CONTINUATION POINT, TARGET POINT, OR LIMIT POINT.

(XC) = THE PREVIOUS CONTINUATION POINT.

(XF) = THE CURRENT CONTINUATION POINT.

(TL) = PREVIOUS VALUE OF TANGENT VECTOR. NOTE THAT THIS CORRESPONDS TO A POINT XL WHICH HAS BEEN DISCARDED. ON A LIMIT POINT RETURN, TL WILL CONTAIN INSTEAD THE TANGENT AT THE LIMIT POINT. ON A TARGET POINT RETURN, TL WILL HAVE BEEN OVERWRITTEN BY THE FUNCTION VALUE AT THE TARGET POINT.

(TC) = THE TANGENT VECTOR AT THE PREVIOUS CONTINUATION POINT.

(FPRYM) = MATRIX STORAGE AREA FOR SETTING UP AND SOLVING THE LINEAR SYSTEMS INVOLVING DFA(X,IP).

ISIZE = USER SET DIMENSION FOR VECTOR RWORK, WHICH MUST BE AT LEAST OF SIZE NVAR*(NVAR+5).

NOMENCLATURE FOR STEP DEPENDENT VARIABLES

THE PROGRAM ACCUMULATES INFORMATION THAT IS ASSOCIATED WITH SEVERAL PREVIOUS CONTINUATION POINTS OR THE STEPS MADE BETWEEN THEM. IN INTERPRETING THE CODE OR ITS OUTPUT, IT IS IMPORTANT TO KNOW WHERE SUCH QUANTITIES APPLY. THE FOLLOWING DESCRIPTION OF SOME OF THE VARIABLES IS VALID ONLY UPON A NORMAL RETURN WITH A CONTINUATION POINT.

THE POINTS 'XLL' AND 'XL' WILL HAVE BEEN DISCARDED BY THE PROGRAM, BUT SOME QUANTITIES ASSOCIATED WITH THEM STILL SURVIVE.

QUANTITIES ASSOCIATED WITH STEP FROM 'XLL' TO 'XL':

HSECLL = SIZE OF SECANT FROM 'XLL' TO 'XL', EUCLIDEAN NORM(XLL-XL)

QUANTITIES ASSOCIATED WITH THE POINT 'XL':

IPL = THE LOCATION OF THE FIRST OR SECOND LARGEST COMPONENT OF THE TANGENT VECTOR AT 'XL'.

TLIM = VALUE OF LIM-TH COMPONENT OF TANGENT VECTOR AT 'XL'.

TL = TANGENT VECTOR AT 'XL', ALTHOUGH LIMIT OR TARGET POINT CALCULATIONS COULD HAVE OVERWRITTEN THIS VECTOR.

QUANTITIES ASSOCIATED WITH INTERVAL FROM 'XL' TO XC:

ALPHLC = THE ANGLE BETWEEN THE TANGENTS AT 'XL' AND XC.

CURVLC = ESTIMATED CURVATURE BETWEEN 'XL' AND XC.

HSECLC = SIZE OF SECANT BETWEEN 'XL' AND XC, EUCLIDEAN NORM(XL-XC)

QUANTITIES ASSOCIATED WITH THE POINT XC:

DETA = BINARY MANTISSA OF DETERMINANT OF DFA(XC,IPL), DIVIDED BY IPL-TH COMPONENT OF TANGENT AT XC.

DIR = SIGN OF DETA, DETERMINES SENSE OF CONTINUATION.

IEXP = BINARY EXPONENT OF DETERMINANT OF DFA(XC,IPL).

IPC = LOCATION OF FIRST OR SECOND LARGEST COMPONENT OF TANGENT VECTOR AT XC.

TC = TANGENT VECTOR AT XC.

TCLIM = VALUE OF LIM-TH COMPONENT OF TANGENT AT XC.

TCIPC = VALUE OF TC(IPC)

QUANTITIES ASSOCIATED WITH THE INTERVAL FROM XC TO XF:

CURVCF = ESTIMATED CURVATURE BETWEEN XC AND XF.

HTANCF = STEPSIZE USED ALONG TANGENT TO GET PREDICTED POINT

C WHICH WAS CORRECTED TO SOLUTION POINT XF. PTCN0421
 C QUANTITIES ASSOCIATED WITH THE POINT XF: PTCN0422
 C CORDIS = SIZE OF THE TOTAL CORRECTION FROM PREDICTED POINT PTCN0423
 C $X = X_C + H \cdot T \cdot \text{TANCF} \cdot TC$ TO CORRECTED POINT XF. PTCN0424
 C NOTE THAT THIS HAS BEEN MODIFIED TO AN 'OPTIMAL' VALUE. PTCN0425
 C CURVXF = A PREDICTED VALUE OF THE CURVATURE AT XF. PTCN0426
 C FNRMXF = MAXIMUM NORM OF FUNCTION VALUE AT XF. PTCN0427
 C FPRYM = DFA(XF,IPC) HAS ACTUALLY BEEN LAST EVALUATED AT THE PTCN0428
 C PENULTIMATE CORRECTOR ITERATE (IF IMOD.NE.1). IT WILL BE PTCN0429
 C EVALUATED AT XF AS SOON AS THE NEXT LOOP BEGINS AND THE PTCN0430
 C TANGENT IS NEEDED. PTCN0431
 C XSTEP = SIZE OF THE LAST CORRECTOR STEP TAKEN IN CONVERGING TO XF. PTCN0432
 C PTCN0433
 C SUBROUTINES IN THIS PACKAGE PTCN0434
 C PTCN0435
 C PTCN0436
 C PTCN0437
 C PTCN0438
 C PTCN0439
 C PITCON(NVAR,LIM,IT,XIT,KSTEP,IPC,H,IRET,IMOD,IPUT, PTCN0440
 C HMAX,HMIN,HFACT,ABSERR,RELERR,RWORK,ISIZE) PTCN0441
 C PTCN0442
 C DRIVING ROUTINE OF CONTINUATION CODE. INITIALIZES INFORMATION, PTCN0443
 C DETERMINES WHETHER LIMIT, TARGET OR CONTINUATION POINT WILL PTCN0444
 C BE SOUGHT THIS STEP, COMPUTES STEPLENGTHS, CONTROLS CORRECTOR PTCN0445
 C PROCESS, AND HANDLES ERROR RETURNS. PTCN0446
 C PTCN0447
 C CORRECT(NVAR,X,IHOLD,WORK,IERR,IMOD,FPRYM,IPUT,ABSERR,RELERR, PTCN0448
 C XSTEP,NEQN,FNRM) PTCN0449
 C PTCN0450
 C USES A FORM OF NEWTON'S METHOD TO SOLVE THE AUGMENTED NONLINEAR PTCN0451
 C SYSTEM $FA(X)=0$ WITH AUGMENTING EQUATION $X(IHOLD)=R$, THAT IS, $X(IHOLD)$ PTCN0452
 C IS HELD FIXED DURING THE CORRECTION PROCESS. PTCN0453
 C PTCN0454
 C TANGNT(NVAR,XC,IPC,TC,IRET,ICALL,FPRYM,IPUT,NEQN,DETA,IEXP) PTCN0455
 C PTCN0456
 C APPLIES ALGORITHM DESCRIBED ABOVE TO SOLVE $DFA(XC,IPL)*TC=E(NVAR)$ PTCN0457
 C AND THEN NORMALIZES TANGENT VECTOR, CORRECTS SIGN, AND SETS PTCN0458
 C IPC AND DIR. PTCN0459
 C PTCN0460
 C ROOT(A,FA,B,FB,C,FC,KOUNT,IFLAG) PTCN0461
 C PTCN0462
 C ROOT FINDER USED TO LOCATE LIMIT POINT. THIS ROUTINE IS A MODIFIED PTCN0463
 C VERSION OF THE FORTRAN FUNCTION ZERO GIVEN IN THE BOOK: PTCN0464
 C 'ALGORITHMS FOR MINIMIZATION WITHOUT DERIVATIVES' PTCN0465
 C BY RICHARD P BRENT, PRENTICE HALL, 1973. PTCN0466
 C PTCN0467
 C SOLVE(NVAR,X,Y,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,IPUT) PTCN0468
 C PTCN0469
 C SETS UP AND SOLVES THE SYSTEM $DFA(X,IP)*Y(OUTPUT)=Y(INPUT)$ PTCN0470
 C WHERE $DFA(X,IP)$ IS THE JACOBIAN OF FA AT X, PTCN0471
 C AND Y IS A RIGHT HAND SIDE SUPPLIED BY THE CALLING ROUTINE. PTCN0472
 C PTCN0473
 C **NOTE** SUBROUTINE SOLVE USES FULL MATRIX STORAGE TO SOLVE THE PTCN0474
 C SYSTEM. THE USER MAY WISH TO REPLACE THIS ROUTINE WITH ONE MORE PTCN0475
 C SUITED TO HIS PROBLEM. PTCN0476
 C PTCN0477
 C PTCN0478
 C PTCN0479
 C PTCN0480
 C PTCN0481
 C PTCN0482
 C PTCN0483
 C FCTN(NVAR,X,FX) PTCN0484
 C EVALUATES THE NVAR-1 COMPONENT FUNCTION FX GIVEN X AN NVAR COMPONENT PTCN0485
 C VECTOR. THIS FUNCTION DESCRIBES THE NONLINEAR SYSTEM. THE AUGMENTING PTCN0486
 C EQUATION IS HANDLED BY THE CONTINUATION PACKAGE. PTCN0487
 C PTCN0488
 C FPRIME(NVAR,X,FPRYM) PTCN0489
 C PTCN0490
 C EVALUATES THE NVAR-1 BY NVAR JACOBIAN MATRIX FPRYM (X)

AT X AND STORES IT IN THE NVAR BY NVAR ARRAY FPRYM,
 SO THAT FPRYM(I,J) CONTAINS (DF(X) (I)/ DX (J)).
 THE LAST ROW OF FPRYM (FOR THE AUGMENTING EQUATION) IS INSERTED
 BY THE ROUTINE SOLVE.

LINPAK ROUTINES USED

LINPAK REFERENCE:
 LINPACK USER'S GUIDE,
 J J DONGARRA, J R BUNCH, C B MOLER AND G W STEWART,
 SOCIETY FOR INDUSTRIAL AND APPLIED MATHEMATICS,
 PHILADELPHIA, 1979.

ISAMAX(N,SX,INCX)
 INTEGER FUNCTION RETURNS THE POSITION OF LARGEST ELEMENT OF SX

SAXPY(N,SA,SX,INCX,SY,INCY)
 SETS VECTOR SY(I) = SA*SX(I)+SY(I)

SCOPY(N,SX,INCX,SY,INCY)
 SETS SY(I)=SX(I)

SDOT(N,SX,INCX,SY,INCY)
 SDOT = SUM(I=1 TO N) SX(I)*SY(I)

SNRM2(N,SX,INCX)
 SNRM2 = EUCLIDEAN NORM OF SX(I)

NOTE SNRM2 HAS MACHINE DEPENDENT CUTOFF CONSTANTS

SSCAL(N,SA,SX,INCX)
 SETS SX(I)=SA*SX(I)

SGEFA(A,LDA,N,IPVT,INFO)
 FACTORS MATRIX A WHOSE LEADING DIMENSION WAS DECLARED AS LDA
 AND WHOSE ACTUAL USED DIMENSION IS N, SETS UP PIVOT INFORMATION
 IN VECTOR IPVT AND WARNS OF ZERO PIVOTS.

SGESL(A,LDA,N,IPVT,B,JOB)
 ACCEPTS OUTPUT OF SGEFA, AND A RIGHT HAND SIDE B, AND SOLVES
 SYSTEM A*X=B, RETURNING X IN B. FOR MODIFIED NEWTON'S METHOD, ONCE
 MATRIX IS FACTORED BY SGEFA, ONLY SGESL IS CALLED FOR SUCCESSIVE
 RIGHT HAND SIDES

LABELED COMMON BLOCKS

/COUNT1/ COUNTS NUMBER OF CALLS FROM ... TO ... AS FOLLOWS:
 ICRSL = CORECT TO SOLVE
 ITNSL = TANGNT TO SOLVE
 NSTCR = PITCON TO CORECT FOR IMPROVED STARTING POINT
 NCNCR = PITCON TO CORECT FOR CONTINUATION POINT
 NTRCR = PITCON TO CORECT FOR TARGET POINTS
 NLHCR = PITCON TO CORECT FOR LIMIT POINT
 NLHRT = PITCON TO ROOT FOR LIMIT POINT

NOTE THAT NSTCR, NCNCR, NTRCR, NLHCR AND NLHRT COUNT THE NUMBER
 OF ITERATIVE STEPS (NEWTON OR ROOTFINDING) AND NOT JUST THE NUMRER
 OF SUBROUTINE CALLS.

/COUNT2/ KEEPS PERFORMANCE AND WORK STATISTICS
 IFEVAL = NUMBER OF CALLS TO FCTN
 IPEVAL = NUMBER OF CALLS TO FPRIME
 ISOLVE = NUMBER OF CALLS TO SOLVE
 NRED = NUMBER OF STEPSIZE REDUCTIONS MADE BEFORE PREDICTOR

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 PTCN0558
 PTCN0559
 PTCN0560

C POINT CONVERGED TO THE NEW CONTINUATION POINT. PTCN0561
 C NRDSUM = TOTAL NUMBER OF STEPSIZE REDUCTIONS PTCN0562
 C KN = NUMBER OF CORRECTOR ITERATION STEPS TAKEN IN MOST RECENT PTCN0563
 C CALL TO CORRECT. PTCN0564
 C KNSUM = TOTAL NUMBER OF CORRECTOR ITERATION STEPS. PTCN0565
 C PTCN0566
 C /OUTPUT/ PTCN0567
 C IWRITE = USER ACCESSIBLE OUTPUT INDICATOR. PTCN0568
 C IWRITE=0, NO OUTPUT PRINTED BY PITCON. PTCN0569
 C IWRITE=1, ERROR MESSAGES PRINTED BY PITCON. PTCN0570
 C IWRITE=2, CERTAIN OUTPUT WILL BE PRINTED BY PITCON. PTCN0571
 C PTCN0572
 C /POINT/ CONTAINS DATA ABOUT THE SOLUTION CURVE PTCN0573
 C DETA = BINARY MANTISSA OF THE DETERMINANT OF THE AUGMENTED JACOBIAN PTCN0574
 C IEXP = BINARY EXPONENT OF THE DETERMINANT OF THE AUGMENTED JACOBIAN PTCN0575
 C CURVCF = ESTIMATED CURVATURE BETWEEN XC AND XF. PTCN0576
 C CORDIS = NORM OF THE CORRECTOR STEP FROM PREDICTED POINT TO CORRECTED PTCN0577
 C POINT, USING MAXIMUM ABSOLUTE VALUE AS THE NORM. PTCN0578
 C THIS QUANTITY IS MODIFIED TO AN 'OPTIMAL' VALUE. PTCN0579
 C ALPHLC = ANGLE BETWEEN OLD AND NEW TANGENTS TL AND TC PTCN0580
 C HSECLC = EUCLIDEAN NORM OF SECANT BETWEEN XL AND XC. PTCN0581
 C FNRNMF = MAXIMUM NORM OF FUNCTION VALUE AT NEW CONTINUATION POINT. PTCN0582
 C PTCN0583
 C /TOL/ PTCN0584
 C EPMACH= SMALLEST NUMBER SUCH THAT $1.0 + \text{EPMACH} \cdot \text{GT} \cdot \text{EPMACH}$ PTCN0585
 C $\cdot \text{SEBETA} \cdot (1 - \text{TAU})$ FOR ROUNDED, TAU-DIGIT ARITHMETIC PTCN0586
 C BASE BETA. TWICE THIS VALUE FOR TRUNCATED ARITHMETIC. PTCN0587
 C THIS IS THE RELATIVE MACHINE PRECISION. PTCN0588
 C EPMACH= $2 \cdot (-27)$ FOR DEC-10. PTCN0589
 C EPSATE= $8 \cdot \text{EPMACH}$ PTCN0590
 C EPSQRT= SQUARE ROOT OF EPMACH PTCN0591
 C PTCN0592
 C PROGRAMMING NOTES PTCN0593
 C PTCN0594
 C THE USER MUST - PTCN0595
 C PTCN0596
 C 1. WRITE SUBROUTINES PTCN0597
 C SUPPLY A CALLING PROGRAM, AND THE TWO ROUTINES FCTN AND FPRIME PTCN0598
 C AS DESCRIBED ABOVE. PTCN0599
 C PTCN0600
 C 2. SET STORAGE AREAS PTCN0601
 C DECLARE A REAL VECTOR RWORK OF SIZE ISIZE, $\text{ISIZE} \cdot \text{GE} \cdot \text{NVAR} \cdot (\text{NVAR} + 5)$ PTCN0602
 C AND AN INTEGER VECTOR IPVT OF SIZE NVAR. PTCN0603
 C PTCN0604
 C 3. PASS CERTAIN NON-DEFAULTABLE VALUES PTCN0605
 C PASS NVAR GREATER THAN ZERO, ISIZE, $\text{GE} \cdot \text{NVAR} \cdot (\text{NVAR} + 5)$ PTCN0606
 C AND SET IRET=0, KSTEP=-1 OR KSTEP=0 ON FIRST CALL. PTCN0607
 C FOR A NEW PROBLEM. PTCN0608
 C PTCN0609
 C THE USER SHOULD - PTCN0610
 C PTCN0611
 C 1. STORE A STARTING POINT XR IN THE FIRST NVAR LOCATIONS OF RWORK PTCN0612
 C BEFORE CALLING PITCON. PTCN0613
 C IF SUCH A VALUE IS NOT GIVEN, THE CODE MAY BE UNABLE TO PRODUCE ONE. PTCN0614
 C PTCN0615
 C 2. CAREFULLY MONITOR THE VALUE OF IRET SO THAT ANY SERIOUS ERROR PTCN0616
 C IS CAUGHT BEFORE ANOTHER CALL IS MADE TO PITCON. PTCN0617
 C PTCN0618
 C 3. CHOOSE A VALUE OF IMOD FOR THE TYPE OF CORRECTOR PROCESS TO PTCN0619
 C BE USED. PTCN0620
 C PTCN0621
 C PTCN0622
 C PTCN0623
 C PTCN0624
 C THE USER MAY - PTCN0625
 C PTCN0626
 C 1. MONITOR THE PASSING OF BIFURCATION POINTS BY SAVING THE OLD PTCN0627
 C VALUE OF DETA AND COMPARING IT TO THE CURRENT VALUE. IF THERE PTCN0628
 C IS A CHANGE IN SIGN, THEN A BIFURCATION POINT HAS BEEN PASSED. PTCN0629
 C PTCN0630

```

C
C 2. ACCESS THE COMMON BLOCKS /COUNT1/ AND /COUNT2/ TO KEEP TRACK
C OF THE AMOUNT OF WORK DONE.
C
C 3. MONITOR THE COMMON BLOCK /POINT/ FOR INFORMATION ABOUT THE
C SOLUTION CURVE.
C
C 4. AT ANY TIME, RESET THE CODE BY PASSING IN KSTEP=-1 OR KSTEP=0.
C THIS ALLOWS THE USER TO CHANGE STEPSIZE, DIRECTION OF CONTINUATION,
C ERROR CONTROLS, OR OTHER PARAMETERS. IT ALSO ENABLES THE USER
C TO RUN UNRELATED PROBLEMS OF DIFFERENT SIZES OR ERROR CONTROLS
C DURING A SINGLE PROGRAM EXECUTION.
C
C THIS SUBROUTINE IS CALLED BY
C USER MAIN PROGRAM
C AND CALLS
C CORRECT
C ROOT
C TANGNT
C FORTRAN ABS
C FORTRAN ACOS
C FORTRAN ALOG
C FORTRAN AMAX1
C FORTRAN AMIN1
C FORTRAN DBLE
C FORTRAN FLOAT
C FORTRAN SIGN
C FORTRAN SIN
C FORTRAN SNGL
C FORTRAN SQRT
C LINPAK JSAMAX
C LINPAK SAXPY
C LINPAK SCOPY
C LINPAK SNRM2
C LINPAK SSCAL
C
C*****
C
C INTEGER IPUT(NVAR)
C REAL RWORK(ISIZE)
C REAL URGE(8),ACOF(12)
C DOUBLE PRECISION DTLIPC,DTCIPC,DADJUS,COSALF
C COMMON /COUNT1/ ICSSL,ITNSL,NSTCR,NCNCR,NTRCR,NLMCR,NLMRT
C COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM
C COMMON /OUTPUT/ IWRITE
C COMMON /POINT/ DETA,IEXP,CURVCF,CORDIS,ALPHLC,HSECLC,FNRMXF
C COMMON /TOL/ EPMACH,EPSATE,EPSRT
C DATA IDONE /0/
C DATA TENM1 /0.1/
C DATA TENM2 /0.01/
C DATA TENM3 /0.001/
C DATA URGE /
C 1 .8735115E+00, .1531947E+00, .3191815E-01, .3339946E-10,
C 2 .4677788E+00, .6970123E-03, .1980863E-05, .1122789E-08/
C DATA ACOF /
C 1 .9043128E+00,-.7075675E+00,-.4667383E+01,-.3677482E+01,
C 2 .8516099E+00,-.1953119E+00,-.4830636E+01,-.9770528E+00,
C 3 .1040061E+01, .3793395E-01, .1042177E+01, .4450706E-01/
C
C*****
C
C 1. PREPARATIONS.
C ON FIRST CALL FOR THIS PROBLEM, INITIALIZE COUNTERS AND VARIABLES,
C CHECK USER INFORMATION AND SET DEFAULTS, AND IF (KSTEP.EQ.-1),
C CHECK NORM OF F(XR) AND CORRECT XR IF NECESSARY.
C ON EACH CALL, IF INPUT IRET HAS NONFATAL VALUE, RESET IRET
C SO THAT CONTINUATION LOOP PICKS UP WHERE IT WAS HALTED.
C
C*****
C

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PTCN0698
PTCN0699
PTCN0700

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C      TERR=0
C      IF (IRET.EQ.-1) IRET=2
C      IF (IRET.EQ.-2.OR.IRET.EQ.-3.OR.IRET.EQ.-4) IRET=1
C      IF (IRET.EQ.-5.OR.IRET.EQ.-6) IRET=0
C
C      IF CODE WAS CALLED AGAIN AFTER FATAL VALUE OF IRET,
C      THEN RETURN WITH ERROR VALUE IRET=-10.
C
C      IF (IRET.LT.0) GO TO 440
C
C      PERFORM ONE-TIME ONLY INITIALIZATIONS
C
C      IF (IDONE.NE.0) GO TO 10
C
C      SET THE MACHINE DEPENDENT VARIABLE EPMACH, THE SMALLEST NUMBER
C      SO THAT (1.0+EPHACH.GT.1.0)
C
C      FOR DEC PDP-10 IN SINGLE PRECISION:
C
C      EPMACH=7.4505806E-9
C
C      FOR IBM 360 OR 370 IN SHORT (SINGLE) PRECISION:
C
C      EPMACH=9.53674E-7
C
C      FOR CDC 6600 OR 7400 IN SINGLE PRECISION:
C
C      EPMACH=7.105427406E-15
C
C      SET EPSATE=8*EPMACH, EPSQRT=SQRT(EPMACH)
C
C      EPSATE=8.0*EPMACH
C      EPSQRT=SQRT(EPMACH)
C      ALFMIN=2.0*ACOS(1.0-EPMACH)
C      IF (KSTEP.LT.-1.OR.KSTEP.GT.0) KSTEP=-1
C      KSTEP0=-2
C      TOONE=1
C
C      PERFORM INITIALIZATIONS AND CHECKS FOR NEW PROBLEM ONLY
C
C      10 IF (KSTEP.GT.0) GO TO 30
C      IF (KSTEP0.EQ.-1.AND.KSTEP.EQ.0) GO TO 30
C      IF (NVAR.LE.1) GO TO 440
C      IF (ISIZE.LT.(NVAR)*NVAR+5) GO TO 440
C      IXR=1
C      JXR=0
C      IXC=IXR+NVAR
C      JXC=JXR+NVAR
C      IXF=IXC+NVAR
C      JXF=JXC+NVAR
C      ITL=IXF+NVAR
C      JTL=JXF+NVAR
C      ITC=ITL+NVAR
C      JTC=JTL+NVAR
C      IFP=ITC+NVAR
C      JFP=JTC+NVAR
C      BETA=0.0
C      TCIPC=0.0
C      CORDIS=0.0
C      CURVCF=0.0
C      HSECLL=0.0
C      HSECLC=0.0
C      XITO=0.0
C      ITO=0
C      NEQN=NVAR-1
C      NRED=0
C      KNSUM=0
C      NRDSUM=0
C      ICRSL=0
C      ITNSL=0

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PTCN0701
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NSTCR=0
NCNCR=0
NTRCR=0
NLNCR=0
NLNRT=0
IFEVAL=0
ISOLVE=0
IPEVAL=0
IF (HMAX.LE.0.0) HMAX=SQRT(FLOAT(NVAR))
IF (HMIN.LE.EPSQRT) HMIN=EPSQRT
HDEF=.5*(HMAX+HMIN)
IF (HFACT.LE.1.0) HFACT=3.0
HRED=1.0/HFACT
IF (ABSERR.LE.0.0) ABSERR=EPSQRT
IF (RELERR.LE.0.0) RELERR=EPSQRT
IF (IPC.LE.0.0.OR.(IPC.GT.NVAR)) IPC=NVAR
IF (LIM.LT.0.0.OR.LIM.GT.NVAR) LIM=0
IF (H.EQ.0.0) H=HDEF
DIR=SIGN(1.0,H)
H=ABS(H)
PTCN0771
PTCN0772
PTCN0773
PTCN0774
PTCN0775
PTCN0776
PTCN0777
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PTCN0840

C
C IF (KSTEP.LT.0) CHECK NORM OF F(XR) AT STARTING POINT,
C IF ACCEPTABLE, RETURN IMMEDIATELY WITH KSTEP=0,
C OTHERWISE APPLY NEWTON'S METHOD, HOLDING VALUE OF
C IPC-TH COMPONENT FIXED.
C
C   IF (KSTEP.GE.0) GO TO 20
C   CALL CORECT(NVAR,RWORK(IXR),IPC,RWORK(ITL),IERR,IMOD,RWORK(IFP),
C   1 IPVT,ABSERR,RELERR,XSTEP,NEON,FNRMXF)
C   NSTCR=NSTCR+KN
C
C IF NO ACCEPTABLE POINT FOUND, ERROR RETURN
C
C   IF (IERR.NE.0) GO TO 400
C   KSTEP0=-1
C   KSTEP=0
C   HTANCF=H
C   GO TO 340
C 20 IF (KSTEP.EQ.0) CALL SCOPY(NVAR,RWORK(IXR),1,RWORK(IXC),1)
C   IF (KSTEP.EQ.0) CALL SCOPY(NVAR,RWORK(IXR),1,RWORK(IXF),1)
C *****
C 2. TARGET POINT CHECK. IF (IT.NE.0) TARGET POINTS ARE SOUGHT.
C CHECK TO SEE IF TARGET COMPONENT IT HAS VALUE XIT LYING
C BETWEEN XC(IT) AND XF(IT). IF SO, GET LINEARLY INTERPOLATED
C STARTING POINT, AND USE NEWTON'S METHOD TO GET TARGET POINT
C *****
C 30 IF (IT.LT.0.OR.IT.GT.NVAR) IT=0
C   IF (IT.EQ.0) GO TO 40
C   IF (ITRET.EQ.1.AND.XIT.EQ.XIT0.AND.IT.EQ.IT0) GO TO 40
C   XCIT=RWORK(JXC+IT)
C   XFIT=RWORK(JXF+IT)
C   IF ((XIT.LT.XCIT).AND.(XIT.LT.XFIT)) GO TO 40
C   IF ((XIT.GT.XCIT).AND.(XIT.GT.XFIT)) GO TO 40
C   DEL=XFIT-XCIT
C   RAT=0.0
C   IF (ABS(DEL).GT.EPSQRT) RAT=(XIT-XCIT)/DEL
C   CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXR),1)
C   CALL SAXPY(NVAR,-1.0,RWORK(IXC),1,RWORK(IXR),1)
C   CALL SBCAL(NVAR,RAT,RWORK(IXR),1)
C   CALL SAXPY(NVAR,1.0,RWORK(IXC),1,RWORK(IXR),1)
C   RWORK(JXR+IT)=XIT
C   CALL CORECT(NVAR,RWORK(IXR),IT,RWORK(ITL),IERR,IMOD,RWORK(IFP),
C   1 IPVT,ABSERR,RELERR,XSTEP,NEON,FNRMXF)
C   NTRCR=NTRCR+KN
C   IT0=IT
C   XIT0=XIT

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      IF (IERR.EQ.0) GO TO 320
      IF (IERR.EQ.-1) GO TO 370
      IF (IERR.EQ.-2) GO TO 360
      IF (IERR.EQ.-3) GO TO 380
C*****
C 3. TANGENT AND LOCAL CONTINUATION PARAMETER CALCULATION. UNLESS THE
C TANGENT AND LIMIT POINT CALCULATIONS WERE ALREADY PERFORMED (BECAUSE
C THE LOOP WAS INTERRUPTED FOR A LIMIT POINT), SET UP AND SOLVE
C THE EQUATION FOR THE TANGENT VECTOR. FORCE THE TANGENT VECTOR TO BE
C OF UNIT LENGTH, AND FORCE THE IPL-COMPONENT TO HAVE THE SAME SIGN AS
C THE IPL-TH COMPONENT OF THE PREVIOUS TANGENT VECTOR, OR (ON FIRST
C STEP) THE SAME SIGN AS THE USER INPUT DIRECTION DIR. SET THE LOCAL
C PARAMETER IPC TO THE LOCATION OF THE LARGEST COMPONENT
C OF THE TANGENT VECTOR, UNLESS A LIMIT POINT IN THAT DIRECTION
C APPEARS TO BE APPROACHING AND ANOTHER CHOICE IS AVAILABLE.
C*****
C 40 IF (IRET.NE.2) GO TO 50
      IRET=0
      GO TO 160
C
C STORE OLD TANGENT IN TL, COMPUTE NEW TANGENT FOR XC
C
C 50 IPL=IPC
      IF (KSTEP.GT.0) CALL SCOPY(NVAR,RWORK(ITC),1,RWORK(ITL),1)
      ICALL=1
      CALL TANGT(NVAR,RWORK(IXF),IPC,RWORK(ITC),IRET,ICALL,RWORK(IFP),
      1 IPUT,NEPN,DETA,IEXP)
      IF (IRET.EQ.-2) GO TO 430
      IF (IRET.EQ.-1) GO TO 410
C
C SUBROUTINE TANGT RETURNED IPC, THE LOCATION OF THE LARGEST COMPONENT
C OF THE TANGENT VECTOR. THIS WILL BE USED FOR THE LOCAL
C PARAMETERIZATION OF THE CURVE UNLESS A LIMIT POINT IN IPC SEEMS
C TO BE COMING. TO CHECK THIS, WE COMPARE TC(IPC)=TC(IPC) AND THE
C SECOND LARGEST COMPONENT TC(JPC)=TC(JPC). IF TCJPC IS NO LESS
C THAN .1 OF TCIPC, AND TC(JPC) IS LARGER THAN TL(JPC),
C WHEREAS TC(IPC) IS LESS THAN TL(IPC), WE WILL RESET THE
C LOCAL PARAMETER IPC:=JPC.
C
      TLIPL=TCIPC
      TCIPC=RWORK(JTC+IPC)
      JPC=IPC
      IF (ABS(TCIPC).GE.ABS(RWORK(JTL+IPC))) GO TO 60
      IF (TLIPL.EQ.0.0) GOTO 60
      RWORK(JTC+IPC)=0.0
      JPC=ISAMAX(NVAR,RWORK(ITC),1)
      TCJPC=RWORK(JTC+JPC)
      RWORK(JTC+IPC)=TCIPC
      IF (ABS(TCJPC).LT.TENM1*ABS(TCIPC)) GO TO 60
      IF (ABS(TCJPC).LT.ABS(RWORK(JTL+JPC))) GOTO 60
      IPC=JPC
      IF (IWRITE.GE.2) WRITE(6,610)
60 TCIPL=RWORK(JTC+IPL)
      DTIPL=DBLE(RWORK(JTL+IPC))
      DETA=DETA/TCIPL
C
C ADJUST SIGN OF TANGENT
C COMPARE THE SIGN OF TC(IPL) WITH SIGN OF TL(IPL)
C (BUT ON FIRST STEP, COMPARE SIGN OF TC(IPL) WITH USER INPUT DIR).
C IF THESE SIGNS DIFFER, CHANGE THE SIGN OF TC TO FORCE AGREEMENT,
C AND THE SIGN OF DETA.
C THEN RECORD DIR:= SIGN OF DETERMINANT = SIGN(DETA).
C
      STLIPL=DIR
      IF (TLIPL.NE.0.0) STLIPL=SIGN(1.0,TLIPL)
      IF (SIGN(1.0,TCIPL).EQ.STLIPL) GO TO 70

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 PTCN0910

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CALL SSCAL(NVAR,-1.0,RWORK(ITC),1)
DETA=-DETA
TCIPL=-TCIPL
70 TCIPC=RWORK(JTC+IPC)
TCJPC=RWORK(JTC+JPC)
DTCTPC=DBLE(TCIPC)
DIR=SIGN(1.0,DETA)
IF (LIM.EQ.0) GO TO 80
TLLIM=TCLIM
TCLIM=RWORK(JTC+LIM)
C
C COMPUTE ALPHLC, THE ANGLE BETWEEN TANGENT AT XL AND TANGENT AT XC
C AND HSECLC, THE EUCLIDEAN NORM OF SECANT FROM XL TO XC.
C
80 IF(KSTEP.LE.0) GO TO 160
COSALF=0.000
DO 90 J=1,NVAR
    COSALF=COSALF+DBLE(RWORK(JTC+J))*DBLE(RWORK(JTL+J))
90 RWORK(JXR+J)=RWORK(JXF+J)-RWORK(JXC+J)
HSECLL=HSECLC
HSECLC=SNRM2(NVAR,RWORK(JXR),1)
ALPHLC=SNGL(COSALF)
IF (ALPHLC.GT.1.0) ALPHLC=1.0
IF (ALPHLC.LT.-1.0) ALPHLC=-1.0
ALPHLC=ACOS(ALPHLC)
IF (WRITE.GE.2) WRITE(6,550)ALPHLC
C
C*****PTCN0938
C 4. LIMIT POINT CHECK. IF (LIM.NE.0) CHECK TO SEE IF
C OLD AND NEW TANGENTS DIFFER IN SIGN OF LIM-TH COMPONENT.
C IF SO, ATTEMPT TO COMPUTE A POINT XR BETWEEN XC AND XF
C FOR WHICH TANGENT COMPONENT VANISHES
C*****PTCN0939
C
C IF (LIM.LE.0.OR.KSTEP.LE.0) GO TO 160
C
C CHECK FOR LIMIT INTERVAL
C
C IF (SIGN(1.0,TCLIM).EQ.SIGN(1.0,TLLIM)) GO TO 160
C
C TEST FOR ACCEPTABLE ENDPOINTS
C
C ATLLM=ABS(TLLIM)
C IF (ATLLM.GT.0.5*ABSERR) GO TO 110
C
C IF XC IS LIMIT POINT, TL ALREADY CONTAINS TANGENT AT XC
C
C 100 CALL SCOPY(NVAR,RWORK(JXC),1,RWORK(JXR),1)
C GO TO 310
C 110 ATCLIM=ABS(TCLIM)
C IF (ATCLIM.GT.0.5*ABSERR) GO TO 130
C 120 CALL SCOPY(NVAR,RWORK(JXF),1,RWORK(JXR),1)
C CALL SCOPY(NVAR,RWORK(ITC),1,RWORK(JTL),1)
C GO TO 310
C
C TEST FOR SMALL INTERVAL
C
C 130 XCLIM=RWORK(JXC+LIM)
C XFLIM=RWORK(JXF+LIM)
C DEL=ABS(XFLIM-XCLIM)
C XABS=AMAX1(ABS(XCLIM),ABS(XFLIM))
C IF (DEL.GT.(ABSERR+RELEERR*XABS)) GO TO 140
C IF (ATLLM.GT.ATCLIM) GO TO 120
C GO TO 100
C
C BEGIN ROOT-FINDING ITERATION WITH INTERVAL (0,1) AND
C FUNCTION VALUES TL(LIM), TC(LIM).
C

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140 KOUNT=0
    A=0.0
    FA=TLLIM
    TSN=TCLIM
    C=1.0
    FC=TCLIM
C
C SET IPLIM TO THE INDEX OF MAXIMUM ENTRY OF SECANT
C (EXCEPT THAT IPLIM MUST NOT EQUAL LIM)
C AND SAVE THE SIGN OF THE MAXIMUM COMPONENT IN DIRLIM
C SO THAT NEW TANGENTS MAY BE PROPERLY SIGNED.
C
    CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(JXR),1)
    CALL SAXPY(NVAR,-1.0,RWORK(IXC),1,RWORK(JXR),1)
    RWORK(JXR+LIM)=0.0
    IPLIM=ISAMAX(NVAR,RWORK(JXR),1)
    DIRLIM=SIGN(1.0,RWORK(JXR+IPLIM))
C
C CALL ROOTFINDER FOR APPROXIMATE ROOT SN, SET X=SN*XF+(1-SN)*XC
C CALL CORRECTOR TO RETURN TO CURVE ON LINE X(IPLIM)=CONSTANT,
C COMPUTE TANGENT THERE, AND SET FUNCTION VALUE TO TANGENT(LIM)
C
150 CALL ROOT(A,FA,SN,TSN,C,FC,KOUNT,IFLAG)
    NLNRT=NLNRT+1
    IF (IFLAG.LT.-1) GO TO 350
    IF (IFLAG.EQ.-1.OR.IFLAG.EQ.0) GO TO 310
    CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(JXR),1)
    CALL SSCAL(NVAR,SN,RWORK(JXR),1)
    SCALER=1.0-SN
    CALL SAXPY(NVAR,SCALER,RWORK(IXC),1,RWORK(JXR),1)
    CALL CORRECT(NVAR,RWORK(JXR),IPLIM,RWORK(ITL),TERR,[MOD,RWORK(TFP)
1 ,IPUT,ABSERR,RELERR,XSTPLM,NEQN,FNRH)
    NLNCR=NLNCR+KN
    IF (TERR.NE.0) GO TO 350
    ICALL=1
    IPT=IPLIM
    CALL TANGNT(NVAR,RWORK(JXR),IPT,RWORK(ITL),IRET,ICALL,
1 RWORK(TFP),IPUT,NEQN,DETLIM,IEXLIM)
    IF (IRET.LT.0) GO TO 350
C
C ADJUST THE SIGN OF THE TANGENT SO THAT THE IPLIM-TH COMPONENT
C HAS THE SAME SIGN AS THE IPLIM-TH COMPONENT OF THE SECANT
C
    IF (DIRLIM.NE.SIGN(1.0,RWORK(JTL+IPLIM)))
1 CALL SSCAL(NVAR,-1.0,RWORK(ITL),1)
C
C SEE IF WE CAN ACCEPT THE NEW POINT BECAUSE TANGENT(LIM) IS SMALL
C OR MUST 'ACCEPT' THE POINT BECAUSE THE VALUES ARE NOT DECREASING
C RAPIDLY ENOUGH, OR IF WE CAN GO ON.
C
    TSHOLD=TSN
    TSN=RWORK(JTL+LIM)
    IF (ABS(TSN).LE.0.5*ABSERR) GO TO 310
    GO TO 150
C
C *****
C 5. STEP LENGTH COMPUTATION. COMPUTE STEPLENGTH HTANCE
C
C THE FORMULAS UNDERLYING THE ALGORITHM ARE
C
C LET
C
C ALPHLC = MAXIMUM OF ARCCOS(TL,TC) AND ALFMIN = 2*ARCCOS(1-EPHACH)
C HSECLC = NORM(XL-XC)
C HSECLL = NORM(XL-XLL)
C ABSIN = ABS(SIN(.5*ALPHLC))
C CURVLC = LAST VALUE OF CURVCF
C CURVCF = 2*ABSIN/HSECLC
C CORDIS = OPTIMIZED CORRECTOR DISTANCE TO CURRENT CONTINUATION POINT.

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C      BUT CORDIS FORCED TO LIE BETWEEN .1*HSECLC AND HSECLC.
C      UNLESS (CORDIS.EQ.0.0), BECAUSE THE PREDICTED POINT WAS
C      IMMEDIATELY ACCEPTED. IN SUCH A CASE, SET HTANCF=HSECLC
C      INSTEAD OF USING FIRST ESTIMATE FOR HTANCF.
C
C      THEN
C
C      CURVXF = CURVCF + HSECLC*(CURVCF-CURVLC)/(HSECLC+HSECLL)
C      BUT CURVXF MUST BE GREATER THAN .001, AND A SIMPLER FORMULA IS USED
C      IF WE DO NOT HAVE DATA AT TWO PREVIOUS POINTS.
C
C      FIRST ESTIMATE: (UNLESS (CORDIS.EQ.0.0) )
C
C      HTANCF = SQRT(2*CORDIS/CURVXF)
C
C      ADJUSTED VALUE:
C
C      HTANCF = HTANCF*(1.0 + HTANCF*(TC(IPC)-TL(IPC))/(2*HSECLC*TC(IPC)))
C
C      READJUSTMENT AND TRUNCATIONS:
C
C      IF STEPSIZE REDUCTION OCCURRED DURING LAST CORRECTOR PROCESS,
C      HTANCF IS FORCED TO BE LESS THAN (HFACT-1)*HSECLC/2.
C
C      HTANCF MUST LIE BETWEEN (HSECLC/HFACT) AND (HSECLC*HFACT).
C
C      HTANCF IS ALWAYS FORCED TO LIE BETWEEN HMIN AND HMAX.
C
C      *****
C
C      CHECK IF DEFAULT STEP MUST BE USED:
C      ON FIRST STEP, USE HTANCF=H.
C      IF PREVIOUS STEP WAS OF SIZE ZERO, USE STEPSIZE HDEF=(HMIN+HMAX)/2
C
C      160 IF (KSTEP.GT.0.AND.HSECLC.GT.0.0) GO TO 170
C          HTANCF=HDEF
C          IF(KSTEP.LE.0)HTANCF=H
C          GO TO 190
C      170 IF (ALPHLC.LT.ALPHMIN)ALPHLC=ALPHMIN
C          ARSIN=ABS(SIN(.5*ALPHLC))
C
C      COMPUTE NEW CURVATURE DATA
C
C          CURVLC=CURVCF
C          CURVCF=2.0*ARSIN/HSECLC
C          CURVXF=CURVCF
C          IF (HSECLL.NE.0.0)
C              1 CURVXF=CURVCF+HSECLC*(CURVCF-CURVLC)/(HSECLC+HSECLL)
C          CURVXF=AMAX1(CURVXF,TEMP3)
C          IF (IWRITE.GE.2)WRITE(6,560)CURVCF,CURVXF
C
C      IF THE CONVERGENCE DISTANCE IS ZERO, SET FIRST ESTIMATE TO HSECLC.
C      OTHERWISE, TRUNCATE CORDIS TO LIE BETWEEN .01*HSECLC AND HSECLC.
C
C          HTANCF=HSECLC
C          IF (CORDIS.EQ.0.0) GO TO 180
C          TEMP=TEMP2*HSECLC
C          CORDIS=AMAX1(CORDIS,TEMP)
C          CORDIS=AMIN1(CORDIS,HSECLC)
C
C      SET HTANCF, THEN ADJUST FOR CURVATURE IN CONTINUATION
C      PARAMETER DIRECTION, THEN TRUNCATE
C
C          HTANCF=SQRT(2.0*CORDIS/CURVXF)
C      180 IF (NREQ.GT.0)HTANCF=AMIN1(HTANCF,(HFACT-1.0)*HSECLC*.5)
C          DADJUS=1.0D0+(1.0D0-DTLIPC/DTCTPC)*DBLE(.5*HTANCF)/DBLE(HSECLC)
C          HTANCF=HTANCF*SNGL(DADJUS)
C          TEMP=HSECLC*NREQ
C          HTANCF=AMAX1(HTANCF,TEMP)
C          TEMP=HSECLC*HFACT

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HTANCF=AMIN1(HTANCF,TEMP)
HTANCF=AMAX1(HTANCF,HMIN)
HTANCF=AMIN1(HTANCF,HMAX)
PTCN1121
PTCN1122
PTCN1123
PTCN1124
C*****PTCN1125
CPTCN1126
C 6. PREDICTION AND CORRECTION STEPS. USING XR=XC+HTANCF*TCPTCN1127
C AS STARTING POINT, CORRECT XR WITH A FULL OR MODIFIED NEWTONPTCN1128
C ITERATION. IF CORRECT FAILS, REDUCE STEPSIZE USED FOR PREDICTORPTCN1129
C POINT, AND TRY AGAIN. CORRECTION WILL ONLY BE ABANDONED IF STEPSIZEPTCN1130
C FALLS BELOW HMIN.PTCN1131
C*****PTCN1132
CPTCN1133
C 190 KSTEP0=KSTEPPTCN1134
C KSTEP=KSTEP+1PTCN1135
C NRED=0PTCN1136
C 200 CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXR),1)PTCN1137
C CALL SAXPY(NVAR,HTANCF,RWORK(ITC),1,RWORK(IXR),1)PTCN1138
C 210 IF(IWRITE.GE.2)WRITE(6,570)HTANCFPTCN1139
C IF(IWRITE.GE.3)WRITE(6,580)(RWORK(JXR+I),I=1,NVAR)PTCN1140
C CALL CORRECT(NVAR,RWORK(IXR),IPC,RWORK(ITL),IERR,IMOD,RWORK(IFP),PTCN1141
C 1 IPVT,ABSERR,RELERR,XSTEP,NEQN,FNRHMF)PTCN1142
C MCNCR=MCNCR+KNPTCN1143
C IF (IERR.EQ.0) GO TO 230PTCN1144
C IF (IERR.EQ.-1) GO TO 420PTCN1145
CPTCN1146
C NO CONVERGENCE, TRY A SMALLER STEPSIZEPTCN1147
CPTCN1148
C HTANCF=HRED*HTANCFPTCN1149
C IF (HTANCF.LT.HMIN) GO TO 390PTCN1150
C NRED=NRED+1PTCN1151
C IF (IERR.EQ.-2) GO TO 220PTCN1152
C GO TO 200PTCN1153
C 220 CALL SAXPY(NVAR,-1.0,RWORK(IXC),1,RWORK(IXR),1)PTCN1154
C CALL SSCAL(NVAR,HRED,RWORK(IXR),1)PTCN1155
C CALL SAXPY(NVAR,1.0,RWORK(IXC),1,RWORK(IXR),1)PTCN1156
C GO TO 210PTCN1157
CPTCN1158
C*****PTCN1159
CPTCN1160
C 7. SUCCESSFUL STEP. STORE INFORMATION BEFORE RETURN.PTCN1161
C UPDATE OLD AND CURRENT CONTINUATION POINTS.PTCN1162
C COMPUTE CORDIS, THE SIZE OF THE CORRECTOR STEP. COMPUTEPTCN1163
C A FACTOR THETA WHICH RESEALS CORDIS TO A VALUE WHICH WOULDPTCN1164
C CORRESPOND TO A DESIRABLE NUMBER OF CORRECTOR STEPSPTCN1165
C (4 FOR FULL NEWTON, 10 FOR MODIFIED NEWTON).PTCN1166
C SEE REFERENCE DEN HEIJER AND RHEINBOLOT, LOC. CIT.PTCN1167
C*****PTCN1168
CPTCN1169
C 230 NRDSUM=NRDSUM+NREDPTCN1170
C IF(NRED.NE.0.AND.IWRITE.GE.2)WRITE(6,590)NREDPTCN1171
CPTCN1172
C COMPUTE CORRECTOR STEP = XC+HTANCF*TC-XFPTCN1173
C SET CORDIS = MAX NORM OF CORRECTOR STEPPTCN1174
CPTCN1175
C CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXC),1)PTCN1176
C CALL SAXPY(NVAR,-1.0,RWORK(IXR),1,RWORK(IXC),1)PTCN1177
C CALL SAXPY(NVAR,HTANCF,RWORK(ITC),1,RWORK(IXC),1)PTCN1178
C IMAX=ISAMAX(NVAR,RWORK(IXC),1)PTCN1179
C CORDIS=ABS(RWORK(JXC+IMAX))PTCN1180
C IF(KN.EQ.0) CORDIS=0.0PTCN1181
CPTCN1182
C MODIFY CORDIS TO A VALUE THAT WOULD CORRESPOND TO THEPTCN1183
C DESIRED NUMBER OF CORRECTOR STEPSPTCN1184
CPTCN1185
C IF(CORDIS.EQ.0.0)GO TO 300PTCN1186
C OMEGA=XSTEP/CORDISPTCN1187
C THETA=0.0PTCN1188
CPTCN1189
CPTCN1190

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C	IF (IMOD.EQ.1) GOTO 260	PTCN1191
C	FULL NEWTON METHOD FOR CORRECTOR STEPS	PTCN1192
C	IF (KN.LE.1) THETA=8.0	PTCN1193
	IF (KN.EQ.4) THETA=1.0	PTCN1194
	IF (THETA.NE.0.0) GO TO 290	PTCN1195
	IF (KN.GT.4) GO TO 240	PTCN1196
	LK=4*KN-7	PTCN1197
	THETA=1.0	PTCN1198
	IF (OMEGA.GE.URGE(LK)) GOTO 290	PTCN1199
	LST=LK	PTCN1200
	IF (OMEGA.GE.URGE(LK+1)) GOTO 250	PTCN1201
	LST=LK+2	PTCN1202
	IF (OMEGA.GE.URGE(LK+2)) GOTO 250	PTCN1203
	THETA=8.0	PTCN1204
	GOTO 290	PTCN1205
240	THETA=0.125	PTCN1206
	IF (KN.GE.7) GOTO 290	PTCN1207
	LK=4*KN-14	PTCN1208
	IF (OMEGA.LE.URGE(LK)) GOTO 290	PTCN1209
	LST=2*KN-1	PTCN1210
250	THETA=ACOF(LST)+ACOF(LST+1)*ALOG(OMEGA)	PTCN1211
	GOTO 290	PTCN1212
C	MODIFIED NEWTON METHOD FOR CORRECTOR STEPS	PTCN1213
C	260 IF (KN.LE.1) THETA=8.0	PTCN1214
	IF (KN.EQ.10) THETA=1.0	PTCN1215
	IF (THETA.NE.0.0) GO TO 290	PTCN1216
	EXPON=FLOAT(KN-1)/FLOAT(KN-10)	PTCN1217
C	AVOID OVERFLOW OR UNDERFLOW BY ANTICIPATING	PTCN1218
C	CUTOFF VALUES OF THETA	PTCN1219
C	IF (KN.GT.10) GO TO 270	PTCN1220
	IF (8.0**EXPON.GT.OMEGA) THETA=8.0	PTCN1221
	IF (.125**EXPON.LT.OMEGA) THETA=.125	PTCN1222
	IF (THETA.NE.0.0) GO TO 290	PTCN1223
	GO TO 280	PTCN1224
270	IF (8.0**EXPON.LT.OMEGA) THETA=8.0	PTCN1225
	IF (.125**EXPON.GT.OMEGA) THETA=.125	PTCN1226
	IF (THETA.NE.0.0) GO TO 290	PTCN1227
280	EXPON=1.0/EXPON	PTCN1228
	THETA=OMEGA**EXPON	PTCN1229
	THETA=AMAX1(THETA,0.125)	PTCN1230
	THETA=AMIN1(THETA,8.0)	PTCN1231
C	SET THE MODIFIED VALUE OF CORDIS	PTCN1232
C	290 CORDIS=THETA*CORDIS	PTCN1233
	IF (IWRITE.GE.2) WRITE(6,400) OMEGA, THETA, CORDIS	PTCN1234
300	CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXC),1)	PTCN1235
	CALL SCOPY(NVAR,RWORK(IXR),1,RWORK(IXF),1)	PTCN1236
	GO TO 340	PTCN1237
C	*****	PTCN1238
C	RETURNS. SET VALUE OF IRET. IF AN ERROR OCCURRED, PRINT	PTCN1239
C	A MESSAGE AS WELL.	PTCN1240
C	*****	PTCN1241
C	RETURN LIMIT POINT	PTCN1242
310	IRET=2	PTCN1243
	RETURN	PTCN1244
C	RETURN WITH TARGET POINT	PTCN1245
C		PTCN1246
		PTCN1247
		PTCN1248
		PTCN1249
		PTCN1250
		PTCN1251
		PTCN1252
		PTCN1253
		PTCN1254
		PTCN1255
		PTCN1256
		PTCN1257
		PTCN1258
		PTCN1259
		PTCN1260

```

C      320 IRET=1
          RETURN
C
C      RETURN WITH CONTINUATION POINT
C
C      330 CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXR),1)
C      340 IRET=0
          H=HTANCF
          RETURN
C
C      ERROR RETURNS
C
C      350 IRET=-1
          IF(IWRITE.GE.1)WRITE(6,450)
          RETURN
C      360 IRET=-2
          IF(IWRITE.GE.1)WRITE(6,460)
          RETURN
C      370 IRET=-3
          IF(IWRITE.GE.1)WRITE(6,470)
          RETURN
C      380 IRET=-4
          IF(IWRITE.GE.1)WRITE(6,480)
          RETURN
C      390 IRET=-5
          IF(IWRITE.GE.1)WRITE(6,490)HTANCF,HMIN
          RETURN
C      400 IRET=-6
          IF(IWRITE.GE.1)WRITE(6,500)
          RETURN
C      410 IRET=-7
          IF(IWRITE.GE.1)WRITE(6,510)
          RETURN
C      420 IRET=-8
          IF(IWRITE.GE.1)WRITE(6,520)
          RETURN
C      430 IRET=-9
          IF(IWRITE.GE.1)WRITE(6,530)
          RETURN
C      440 IRET=-10
          IF(IWRITE.GE.1)WRITE(6,540)NVAR,ISIZE
          RETURN
C      450 FORMAT(26H0LIMIT POINT FINDER FAILED)
C      460 FORMAT(50HOCORECT, SEEKING TARGET POINT, TOOK TOO MANY STEPS)
C      470 FORMAT(50HOCORECT, SEEKING TARGET, CALLED SOLVE WHICH FAILED)
C      480 FORMAT(45HOCORECT, SEEKING TARGET, FAILED WITH RAD STEP)
C      490 FORMAT(10H0STEP SIZE ,F12.7,15H LESS THAN HMIN,F12.7)
C      500 FORMAT(42H0NORM OF F(X) IS TOO LARGE ON INITIAL CALL)
C      510 FORMAT(33H0SOLVE FAILED IN CALL FROM TANGNT)
C      520 FORMAT(33H0SOLVE FAILED IN CALL FROM CORECT)
C      530 FORMAT(23H0TANGENT VECTOR IS ZERO)
C      540 FORMAT(26H0UNACCEPTABLE INPUT NVAR=,I10,7H ISIZE=,I10)
C      550 FORMAT(36H ANGLE BETWEEN OLD AND NEW TANGENTS=,F12.5)
C      560 FORMAT(9H CURVCF =,E14.6,9H CURVXF =,E14.6)
C      570 FORMAT(16H USING STEP SIZE=,F12.5)
C      580 FORMAT(12H PREDICTED X/1X,5F12.5)
C      590 FORMAT(1H ,12,16H STEP REDUCTIONS)
C      600 FORMAT(7H OMEGA=,F12.5,7H THETA=,F12.5,9H NEW RAD=,F12.5)
C      610 FORMAT(31H TANGNT ANTICIPATES LIMIT POINT)
C
C*****
C
C      END

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PTCN1261
PTCN1262
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PTCN1322
PTCN1323
PTCN1324

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SUBROUTINE CORECT(NVAR,X,IHOLD,WORK,IERR,IMOD,FPRYM,IPUT,
1 ABSERR,RELERR,XSTEP,NEQN,FNRN)
C
C*****
C
C SUBROUTINE CORECT PERFORMS THE CORRECTOR ITERATIONS ON A STARTING
C POINT. THE CORRECTION METHOD IS EITHER FULL (IMOD=0)
C OR MODIFIED (IMOD=1) NEWTON'S METHOD. FOR MODIFIED NEWTON'S
C METHOD, THE JACOBIAN IS TO BE EVALUATED ONLY AT THE STARTING POINT.
C IF B IS THE VALUE OF X(IHOLD) FOR THE INPUT STARTING POINT,
C THEN THE AUGMENTING EQUATION IS  $X(IHOLD)=B$ ,
C THAT IS, THE IHOLD-TH COMPONENT OF X IS TO BE HELD FIXED.
C THE AUGMENTED SYSTEM TO BE SOLVED IS THEN  $DFA(X,IHOLD)*DELTA=FA(X)$ 
C
C INPUT
C X = THE STARTING POINT FOR THE CORRECTOR ITERATION.
C IHOLD = COMPONENT OF X THAT WILL NOT BE CHANGED DURING ITERATION
C IMOD = FLAG FOR TYPE OF NEWTON'S METHOD TO BE USED.
C WHEN IMOD=0, JACOBIAN IS TO BE EVALUATED AT EVERY
C CORRECTOR ITERATE. KNMAX IS SET TO 10
C IF IMOD=1, THE JACOBIAN IS ONLY EVALUATED AT THE STARTING
C POINT, AND KNMAX IS SET TO 20.
C
C OUTPUT
C X = SOLUTION VECTOR ON A SUCCESSFUL CALL TO CORECT.
C WORK = THE RESIDUAL F(X), AFTER A SUCCESSFUL CALL TO CORECT.
C IERR = THE RETURN FLAG WITH THE FOLLOWING VALUES
C -2 MAXIMUM NUMBER OF CORRECTOR ITERATIONS WERE TAKEN.
C -1 ERROR RETURN FROM SOLVE CALLED BY CORECT.
C 0 SUCCESSFUL CORRECTION. VECTOR X RETURNED SATISFIES
C  $ABS(F(X)).LE.ABSERR$ 
C 1 CORRECTOR STEP WAS UNACCEPTABLE, CORRECTION FAILED.
C KN = THE NUMBER OF CORRECTOR ITERATIONS TAKEN ON THIS CALL
C
C THIS SUBROUTINE IS CALLED BY
C PITCON
C AND CALLS
C SOLVE
C FORTRAN ABS
C LINPAK ISAMAX
C LINPAK SAXPY
C USER FCTN
C
C*****
C
C REAL X(NVAR),WORK(NVAR),FPRYM(NVAR,NVAR)
C INTEGER IPUT(NVAR)
C COMMON /COUNT1/ ICRSL,ITNSL,NSTCR,NCNCR,NTRCR,NLMCR,NLMRT
C COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM
C COMMON /OUTPUT/ IWRITE
C COMMON /TOL/ EPMACH,EPSATE,EPSRT
C
C INITIALIZE
C
C KN=0
C KNMAX=10
C IF(IMOD.EQ.1)KNMAX=20
C IERR=0
C FMP=2.0
C ICALL=1
C XSTEP=0.0
C CALL FCTN(NVAR,X,WORK)
C IFEVAL=IFEVAL+1
C IMAX=ISAMAX(NEQN,WORK,1)
C FNRN=ABS(WORK(IMAX))
C WORK(NVAR)=0.0
C
C STRICTER ABSERR TEST ON STARTING POINT
C
C IF (FNRN.LE.0.5*ABSERR) GO TO 60

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CRCT0001
 CRCT0002
 CRCT0003
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 CRCT0006
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 CRCT0064
 CRCT0065
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 CRCT0068
 CRCT0069
 CRCT0070

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C
C  ITERATION LOOP
C
      DO 20 I=1, KNMAX
        KN=I
        CALL SOLVE(NVAR,X,WORK,IMOLD,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,
1      IPVT)
        ICRSL=ICRSL+1
        IF(IMOD.EQ.1)ICALL=0
        ISOLVE=ISOLVE+1
        IF(IERR.NE.0) GO TO 50
        FNRML=FNRM
        XSTEPL=XSTEP
        CALL SAXPY(NVAR,-1.0,WORK,1,X,1)
        IMAX=ISAMAX(NVAR,WORK,1)
        XSTEP=ABS(WORK(IMAX))
        IMAX=ISAMAX(NVAR,X,1)
        XNRM=ABS(X(IMAX))
        CALL FCTN(NVAR,X,WORK)
        IFEVAL=IFEVAL+1
        IMAX=ISAMAX(NVRN,WORK,1)
        FNRM=ABS(WORK(IMAX))
        WORK(NVAR)=0.0
C
C  ACCEPTANCE TEST
C
        IF (FNRM.IE.EPSATE) GO TO 60
        IF (FNRM.GT.ABSERR) GO TO 10
        IF (XSTEP.LE.(ABSERR+RELEERR*XNRM)) GO TO 60
C
C  REJECTION TEST
C
        10      IF (KN.GT.1.AND.XSTEP.GT.(FMP*XSTEPL)) GO TO 30
        IF (FNRM.GT.(FMP*FNRML)) GO TO 30
        20      FMP=1.05
        GO TO 40
C
C  UNSUCCESSFUL STEP
C
        30 IERR=-3
        IF(IWRITE.EQ.2)WRITE(6,120)
        GO TO 70
C
C  MAXIMUM NUMBER OF CORRECTOR STEPS REACHED
C
        40 IERR=-2
        IF(IWRITE.EQ.2)WRITE(6,110)
        GO TO 70
C
C  ERROR RETURN IN SOLVE
C
        50 IERR=-1
        IF(IWRITE.EQ.2)WRITE(6,100)
        GO TO 70
C
C  SUCCESSFUL STEP
C
        60 IERR=0
        70 KNSUM=KNSUM+KN
        IF(IWRITE.EQ.2)WRITE(6,80) KN,XSTEP
        IF(IWRITE.EQ.2)WRITE(6,90)IMOLD
        RETURN
        80 FORMAT(13H CORECT TOOK ,I2,21H STEPS, LAST ONE WAS ,E12.5)
        90 FORMAT(14H CORECT IMOLD=,I3)
        100 FORMAT(31HOSOLVE FAILED, CALLED BY CORECT)
        110 FORMAT(25HOTOO MANY CORRECTOR STEPS)
        120 FORMAT(24HOCORRECTOR STEP REJECTED)
C
C *****
C
      END

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CRCT0071
CRCT0072
CRCT0073
CRCT0074
CRCT0075
CRCT0076
CRCT0077
CRCT0078
CRCT0079
CRCT0080
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CRCT0115
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CRCT0125
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CRCT0140
CRCT0141

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SUBROUTINE TANGNT(NVAR,X,IP,TAN,IRET,ICALL,FPRYM,IPUT,NEQN,DETA,  TNGN0001
1 IEXP)  TNGN0002
C*****  TNGN0003
C  TNGN0004
C  TNGN0005
C  SURROUTINE TANGNT COMPUTES THE UNIT TANGENT VECTOR TO THE SOLUTION  TNGN0006
C  CURVE OF THE UNDERDETERMINED NONLINEAR SYSTEM  $FX = 0$ . THE  TNGN0007
C  TANGENT VECTOR TAN IS THE SOLUTION OF THE LINEAR SYSTEM  TNGN0008
C  TNGN0009
C  DFA(X,IPL)*TAN = E(NVAR)  TNGN0010
C  TNGN0011
C  WHERE DFA(X,IPL) IS THE NVAR BY NVAR MATRIX WHOSE FIRST NVAR-1 ROWS  TNGN0012
C  ARE DFX/DX (X), THE DERIVATIVE OF FX EVALUATED AT X, AND WHOSE LAST  TNGN0013
C  ROW IS (E(IPL)) TRANSPOSE, THE NVAR COMPONENT EUCLIDEAN COORDINATE  TNGN0014
C  VECTOR WITH 1 IN THE IPL-TH POSITION AND ZEROS ELSEWHERE. E(NVAR) IS  TNGN0015
C  THE NVAR COMPONENT EUCLIDEAN COORDINATE VECTOR WITH ONE IN THE  TNGN0016
C  LAST COMPONENT.  TNGN0017
C  THE TANGENT VECTOR IS THEN NORMALIZED AND ITS SIGN ADJUSTED.  TNGN0018
C  TNGN0019
C  INPUT  TNGN0020
C  NVAR = THE NUMBER OF VARIABLES  TNGN0021
C  X = THE CURRENT CONTINUATION POINT  TNGN0022
C  IP = CONTINUATION COMPONENT SET ON LAST STEP  TNGN0023
C  TNGN0024
C  OUTPUT  TNGN0025
C  TAN = THE UNIT TANGENT VECTOR IN CONTINUATION DIRECTION AT X  TNGN0026
C  DETA = BINARY MANTISSA OF DETERMINANT OF JACOBIAN DFA(X,IPL)  TNGN0027
C  IEXP = BINARY EXPONENT OF THE DETERMINANT OF JACOBIAN DFA(X,IPL)  TNGN0028
C  IP = LOCATION OF LARGEST COMPONENT OF TANGENT VECTOR TAN  TNGN0029
C  CANDIDATE FOR NEW CONTINUATION COMPONENT  TNGN0030
C  TNGN0031
C  THIS SUBROUTINE IS CALLED BY  TNGN0032
C  PITCON  TNGN0033
C  AND CALLS  TNGN0034
C  SOLVE  TNGN0035
C  LINPAK ISAMAX  TNGN0036
C  LINPAK SNRM2  TNGN0037
C  LINPAK SSCAL  TNGN0038
C  TNGN0039
C*****  TNGN0040
C  TNGN0041
C  REAL X(NVAR),TAN(NVAR),FPRYM(NVAR,NVAR)  TNGN0042
C  INTEGER IPUT(NVAR)  TNGN0043
C  COMMON /COUNT1/ ICNLS,ITNSL,NSTCR,NCNCR,NTRCR,NLHCR,NLHRT  TNGN0044
C  COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM  TNGN0045
C  COMMON /OUTPUT/ IWRITE  TNGN0046
C  TNGN0047
C  COMPUTE TANGENT VECTOR  TNGN0048
C  TNGN0049
C  DO 10 I=1,NEQN  TNGN0050
10  TAN(I)=0.0  TNGN0051
  TAN(NVAR)=1.0  TNGN0052
  IERR=0  TNGN0053
  CALL SOLVE(NVAR,X,TAN,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,  TNGN0054
1 IPUT)  TNGN0055
  ITNSL=ITNSL+1  TNGN0056
  ISOLVE=ISOLVE+1  TNGN0057
  IF (IERR.NE.0) IRET=-1  TNGN0058
  IF (IRET.LT.0) RETURN  TNGN0059
C  TNGN0060
C  OBTAIN EUCLIDEAN NORM OF TANGENT VECTOR  TNGN0061
C  TNGN0062
C  IP=ISAMAX(NVAR,TAN,1)  TNGN0063
  TNORM=SNRM2(NVAR,TAN,1)  TNGN0064
  IF (TNORM.EQ.0.0) IRET=-2  TNGN0065
  IF (IRET.LT.0) RETURN  TNGN0066
C  TNGN0067
C  NORMALIZE THE VECTOR  TNGN0068
C  TNGN0069
  SCALER=1.0/TNORM  TNGN0070
  CALL SSCAL(NVAR,SCALER,TAN,1)  TNGN0071
  RETURN  TNGN0072
C  TNGN0073
C*****  TNGN0074
C  TNGN0075
C  END  TNGN0076

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C      SUBROUTINE ROOT(A,FA,B,FB,C,FC,KOUNT,IFLAG)
C      C*****
C      SUBROUTINE ROOT SEEKS A ROOT OF THE EQUATION F(X)=0.0,
C      GIVEN A STARTING INTERVAL (A,C) ON WHICH F CHANGES SIGN.
C      ON FIRST CALL TO ROOT, THE INTERVAL AND FUNCTION VALUES
C      FA AND FC ARE FED IN AND AN APPROXIMATION B FOR THE ROOT IS RETURNED.
C      BEFORE EACH SUBSEQUENT CALL, THE USER EVALUATES FB=F(B), AND THE
C      PROGRAM TRIES TO RETURN A BETTER APPROXIMATION B.
C      THIS PROGRAM IS BASED ON THE FORTRAN FUNCTION ZERO
C      GIVEN IN THE BOOK:
C      'ALGORITHMS FOR MINIMIZATION WITHOUT DERIVATIVES'
C      BY RICHARD P. BRENT, PRENTICE HALL, INC, 1973
C      THE MODIFICATIONS WERE DONE BY JOHN BURKARDT.
C      ON INPUT:
C      A      - IS ONE ENDPOINT OF AN INTERVAL IN WHICH F CHANGES SIGN.
C      FA     - THE VALUE OF F(A). THE USER MUST EVALUATE F(A) BEFORE FIRST
C      B      - ON FIRST CALL, B SHOULD NOT BE SET BY THE USER.
C      ON SUBSEQUENT CALLS, B SHOULD NOT BE CHANGED
C      FROM ITS OUTPUT VALUE, THE CURRENT APPROXIMANT
C      TO THE ROOT.
C      FB     - ON FIRST CALL, FB SHOULD NOT BE SET BY THE USER.
C      THEREAFTER, THE USER SHOULD EVALUATE THE FUNCTION
C      AT THE OUTPUT VALUE B, AND RETURN FB=F(B).
C      C      - IS THE OTHER ENDPOINT OF THE INTERVAL IN WHICH
C      F CHANGES SIGN. NOTE THAT THE PROGRAM WILL RETURN
C      IMMEDIATELY WITH AN ERROR FLAG IF FC*FA.GT.0.0.
C      FC     - THE VALUE OF F(C). THE USER MUST EVALUATE F(C) BEFORE FIRST
C      CALL ONLY. THEREAFTER THE PROGRAM SETS FC.
C      KOUNT  - A COUNTER FOR THE NUMBER OF CALLS TO ROOT. KOUNT
C      SHOULD BE SET TO ZERO ON THE FIRST CALL FOR A GIVEN
C      ROOT PROBLEM.
C      IFLAG  - AN ERROR RETURN FLAG WHOSE INPUT VALUE IS IMMATERIAL.
C      ON RETURN FROM A CALL TO ROOT
C      A      - ONE ENDPOINT OF CHANGE OF SIGN INTERVAL.
C      FA     - THE VALUE OF F(A).
C      B      - CURRENT APPROXIMATION TO THE ROOT. BEFORE ANOTHER
C      CALL TO ROOT, EVALUATE F(B).
C      FB     - FB WILL BE OVERWRITTEN BY THE USER BEFORE ANOTHER
C      CALL. ITS VALUE ON RETURN IS ONE OF FA, FB OR FC.
C      C      - OTHER ENDPOINT OF CHANGE IN SIGN INTERVAL.
C      FC     - THE VALUE OF F(C).
C      KOUNT  - CURRENT NUMBER OF CALLS TO ROOT.
C      IFLAG  - PROGRAM RETURN FLAG:
C      IFLAG=-2 MEANS THAT ON FIRST CALL, FA*FC.GT.0.0.
C      THIS IS AN ERROR RETURN, SINCE A BRACKETING
C      INTERVAL SHOULD BE SUPPLIED ON FIRST CALL.
C      IFLAG=-1 MEANS THAT THE CURRENT BRACKETING INTERVAL
C      WHOSE ENDPOINTS ARE STORED IN A AND C
C      IS SO SMALL (LESS THAN 4*EPMACH*ABS(B)+EPMACH)
C      THAT B SHOULD BE ACCEPTED AS THE ROOT.
C      THE FUNCTION VALUE F(B) IS STORED IN FB.
C      IFLAG= 0 MEANS THAT THE INPUT VALUE FB IS EXACTLY
C      ZERO, AND B SHOULD BE ACCEPTED AS THE ROOT.
C      IFLAG.GT.0 MEANS THAT THE CURRENT APPROXIMATION TO
C      THE ROOT IS CONTAINED IN B. IF A BETTER
C      APPROXIMATION IS DESIRED, SET FB=F(B)
C      AND CALL ROOT AGAIN. THE VALUE OF IFLAG INDICATES
C      THE METHOD THAT WAS USED TO PRODUCE B.
C      IFLAG= 1 BISECTION WAS USED.

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C          IFLAG= 2 LINEAR INTERPOLATION (SECANT METHOD).
C          IFLAG= 3 INVERSE QUADRATIC INTERPOLATION.
C
C LOCAL VARIABLES INCLUDE:
C
C EPMACH- SMALLEST POSITIVE NUMBER SUCH THAT 1.0+EPMACH.GT.1.0
C          .5*BETA*(1-TAU) FOR ROUNDED, TAU-DIGIT ARITHMETIC
C          BASE BETA. TWICE THAT VALUE FOR TRUNCATED ARITHMETIC.
C          THIS IS THE RELATIVE MACHINE PRECISION.
C HALFBC- SIGNED HALFWIDTH OF INTERVAL. DURING SEGMENT 3, THE
C          CHANGE OF SIGN INTERVAL IS (B,C) OR (C,R). THE MIDPOINT
C          OF THAT INTERVAL IS XMID=B+HALFBC, REGARDLESS OF ORIENTATION.
C SDEL1 - SIZE OF CHANGE IN SIGN INTERVAL.
C SDEL2 - PREVIOUS VALUE OF SDEL1.
C SDEL3 - PREVIOUS VALUE OF SDEL2.
C SDEL4 - PREVIOUS VALUE OF SDEL3.
C STEP - THE NEW ROOT IS COMPUTED AS A CORRECTION TO B OF THE
C        FORM B(NEW)=B(OLD)+STEP.
C TOLER - A NUMBER WE ACCEPT AS 'SMALL' WHEN EXAMINING INTERVAL
C         SIZE OR STEP SIZE. TOLER=2.0*EPMACH*ABS(B) + EPMACH IS
C         A MINIMUM BELOW WHICH WE WILL NOT ALLOW SUCH VALUES TO FALL.
C THIS SUBROUTINE IS CALLED BY
C PITCON
C AND CALLS
C FORTRAN ABS
C FORTRAN SIGN
C
C *****
C REAL A,B,C,FA,FR,FC,STEP,TOLER,P,Q,R,S
C COMMON /TOL/ EPMACH,EPSATE,EPSQRT
C
C SEGMENT 1: FIRST CALL HANDLED SPECIALLY. DO BOOKKEEPING.
C
C SET CERTAIN VALUES ONLY FOR INITIAL CALL WITH KOUNT=0
C
C IF (KOUNT.GT.0) GO TO 10
C IF (FA.GT.0.0.AND.FC.GT.0.0) GO TO 110
C IF (FA.LT.0.0.AND.FC.LT.0.0) GO TO 110
C KOUNT=1
C SDEL1=2.0*ABS(C-A)
C SDEL2=2.0*SDEL1
C SDEL3=2.0*SDEL2
C B=C
C FB=FC
C GO TO 20
C
C ON EVERY CALL, INCREMENT COUNTER
C
C 10 KOUNT=KOUNT+1
C
C RETURN IF HIT MACHINE ZERO FOR F(B)
C
C IF(FB.EQ.0.0) GO TO 90
C
C SEGMENT 2: REARRANGE POINTS AND FUNCTION VALUES IF
C NECESSARY SO THAT FB*FC.LT.0.0, AND SO THAT
C ABS(FB).LT.ABS(FC)
C
C IF((FB.LE.0.0).AND.(FC.GT.0.0)) GO TO 30
C IF((FB.GT.0.0).AND.(FC.LE.0.0)) GO TO 30
C
C FB AND FC ARE OF SAME SIGN.
C (ROOT CHANGED SIGN)
C OVERWRITE C WITH VALUE OF A
C
C 20 C=A
C FC=FA

```

ROOT0071
 ROOT0072
 ROOT0073
 ROOT0074
 ROOT0075
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 ROOT0100
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 ROOT0125
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 ROOT0134
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 ROOT0136
 ROOT0137
 ROOT0138

```

C
C IF NECESSARY, SET A:=B, B:=C, C:=B
C TO ENSURE THAT ABS(FB).LE.ABS(FC)
C
30 IF(ABS(FC).GE.ABS(FB)) GO TO 40
  A=B
  B=C
  C=A
  FA=FB
  FB=FC
  FC=FA
C
C SEGMENT 3: CHECK FOR ACCEPTANCE BECAUSE OF SMALL INTERVAL
C CURRENT CHANGE IN SIGN INTERVAL IS (C,B) OR (B,C).
C
40 TOLER=2.0*EPMACH*ABS(B)+EPMACH
  HALFRC=0.5*(C-B)
  SDEL4=SDEL3
  SDEL3=SDEL2
  SDEL2=SDEL1
  SDEL1=ABS(C-B)
  IF(ABS(HALFRC).LE.TOLER) GO TO 100
C
C SEGMENT 4: COMPUTE NEW APPROXIMANT TO ROOT OF THE FORM
C B(NEW)=B(OLD)+STEP.
C METHODS AVAILABLE ARE LINEAR INTERPOLATION
C INVERSE QUADRATIC INTERPOLATION
C AND BISECTION.
C
  IF(ABS(FB).GE.ABS(FA))GO TO 70
  IF(A.NE.C) GO TO 50
C
C ATTEMPT LINEAR INTERPOLATION IF ONLY TWO POINTS AVAILABLE
C COMPUTE P AND Q FOR APPROXIMATION B(NEW)=B(OLD)+P/Q
C
  IFLAG=2
  S=FB/FA
  P=2.0*HALFRC*S
  Q=1.0-S
  GO TO 60
C
C ATTEMPT INVERSE QUADRATIC INTERPOLATION IF THREE POINTS AVAILABLE
C COMPUTE P AND Q FOR APPROXIMATION B(NEW)=B(OLD)+P/Q
C
50 IFLAG=3
  S=FB/FA
  Q=FA/FC
  R=FB/FC
  P=S*(2.0*HALFRC*Q*(R-R)-(B-A)*(R-1.0))
  Q=(Q-1.0)*(R-1.0)*(S-1.0)
C
C CORRECT THE SIGNS OF P AND Q
C
60 IF(P.GT.0.0)Q=-Q
  P=ABS(P)
C
C IF P/Q IS TOO LARGE, GO BACK TO BISECTION
C
  IF(8.0*SDEL1.GT.SDEL4) GO TO 70
  IF (P.GE.1.5*ABS(HALFRC*Q)-ABS(TOLER*Q)) GO TO 70
  STEP=P/Q
  GO TO 80
C
C PERFORM BISECTION:
C IF ABS(FB).GE.ABS(FA)
C OR INTERPOLATION IS UNSAFE (P/Q IS LARGE)
C OR IF THREE CONSECUTIVE STEPS HAVE NOT DECREASED
C THE SIZE OF THE INTERVAL BY A FACTOR OF 8.0
C
70 IFLAG=1
  STEP=HALFRC
  GO TO 80

```

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ROOT0139
ROOT0140
ROOT0141
ROOT0142
ROOT0143
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ROOT0194
ROOT0195
ROOT0196
ROOT0197
ROOT0198
ROOT0199
ROOT0200
ROOT0201
ROOT0202
ROOT0203
ROOT0204
ROOT0205
ROOT0206
ROOT0207
ROOT0208
ROOT0209
ROOT0210

```

C	SEGMENT 5: VALUE OF STEP HAS BEEN COMPUTED.	ROOT0211
C	UPDATE INFORMATION: A:=B, FA:=FB, B:=B+STEP.	ROOT0212
C	CHANGE IN SIGN INTERVAL IS NOW (A,C) OR (C,A).	ROOT0213
C		ROOT0214
	80 A=B	ROOT0215
	FA=FB	ROOT0216
	IF(ABS(STEP).LE.TOLER) STEP=SIGN(TOLER,HALFRC)	ROOT0217
	B=B+STEP	ROOT0218
	RETURN	ROOT0219
C		ROOT0220
C	SPECIAL RETURNS	ROOT0221
C		ROOT0222
C	INPUT POINT B IS EXACT ROOT	ROOT0223
C		ROOT0224
C	90 IFLAG=0	ROOT0225
	RETURN	ROOT0226
C		ROOT0227
C	CHANGE IN SIGN INTERVAL IS OF SIZE LESS THAN 4*EPMACH*ABS(B)+EPMACH	ROOT0228
C	INTERVAL RETURNED AS (B,C) OR (C,B).	ROOT0229
C	ACCEPT B AS ROOT WITH RESIDUAL F(B) STORED IN FB.	ROOT0230
C		ROOT0231
	100 IFLAG=-1	ROOT0232
	A=B	ROOT0233
	FA=FB	ROOT0234
	RETURN	ROOT0235
C		ROOT0236
C	CHANGE OF SIGN CONDITION VIOLATED	ROOT0237
C		ROOT0238
	110 IFLAG=-2	ROOT0239
	KOUNT=0	ROOT0240
	RETURN	ROOT0241
C		ROOT0242
C	*****	ROOT0243
C		ROOT0244
	END	ROOT0245
		ROOT0246

```

SUBROUTINE SOLVE(NVAR,X,Y,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,
1 IPVT)
C*****
C THIS SUBROUTINE IS CALLED BY
C   CORECT
C   TANGNT
C AND CALLS
C   FORTRAN ABS
C   LINPAK SGEFA
C   LINPAK SGESL
C   USER FPRIME
C
C THIS SUBROUTINE SOLVES THE LINEAR SYSTEM DFA(X,IP)*YOUT = YIN
C WHERE DFA(X,IP) IS THE (NVAR)*X(NVAR) MATRIX WHOSE FIRST NVAR - 1
C ROWS ARE THE JACOBIAN COMPUTED BY FPRIME, AND WHOSE LAST
C ROW IS ALL 0 EXCEPT FOR A 1 IN THE IP-TH COMPONENT.
C
C YIN IS THE NVAR COMPONENT VECTOR Y ON INPUT, AND THE SOLUTION
C VECTOR YOUT IS RETURNED IN Y ON OUTPUT AFTER A SUCCESSFUL
C SETUP AND SOLUTION.
C
C **NOTE** SUBROUTINE SOLVE USES FULL MATRIX STORAGE TO SOLVE THE
C LINEAR SYSTEM. THE USER MAY WISH TO REPLACE THIS ROUTINE WITH
C ONE MORE SUITED TO HIS PROBLEM.
C
C DETA  BINARY MANTISSA OF THE DETERMINANT OF JACOBIAN DFA(X,IP)
C IEXP  BINARY EXPONENT OF THE DETERMINANT OF JACOBIAN DFA(X,IP)
C IMOD  NEWTON METHOD FLAG.
C       IMOD=0, JACOBIAN IS TO BE EVALUATED FOR EVERY CORRECTOR STEP
C           AND EVERY TANGENT CALCULATION
C       IMOD=1, JACOBIAN IS TO BE EVALUATED ONLY FOR FIRST CORRECTOR
C           STEP, AND EVERY TANGENT CALCULATION
C ICALL  SET UP FLAG.
C        IF (ICALL.EQ.0.AND.IMOD.NE.0) DON'T RE-EVALUATED JACOBIAN
C INFO  OUTPUT FROM SGEFA. IF INFO.NE.0, SGEFA FOUND A ZERO
C       PIVOT WHEN ELIMINATING INFO-TH VARIABLE.
C IERR  RETURN FLAG, 0 MEANS SUCCESSFUL SOLUTION, 1 MEANS FAILURE
C NVAR  THE NUMBER OF VARIABLES IN THE NONLINEAR SYSTEM
C X     THE POINT AT WHICH TO EVALUATE FPRYM
C Y     THE RIGHT HAND SIDE ON INPUT, THE SOLUTION
C       ON OUTPUT
C FPRYM ARRAY WHERE DFA(X,IP) IS TO BE STORED.
C IPVT  INTEGER WORK SPACE FOR PIVOT ROW SWITCHES DEMANDED BY SGEFA
C IP    THE VARIABLE USED IN THE AUGMENTING EQUATION THAT IS OF THE
C       FORM X(IP)=B. HENCE THE LAST ROW OF DFA(X,IP) IS ALL
C       ZERO EXCEPT FOR A 1.0 IN THE IP-TH COLUMN.
C*****
C REAL X(NVAR),Y(NVAR),FPRYM(NVAR,NVAR)
C INTEGER IPVT(NVAR)
C COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM
C
C DEPENDING ON VALUES OF ICALL AND IMOD, EITHER SET UP
C AUGMENTED JACOBIAN, DECOMPOSE INTO L-U FACTORS, AND GET DETERMINANT,
C OR USE CURRENT FACTORED JACOBIAN WITH NEW RIGHT HAND SIDE.
C
C IF (ICALL.EQ.0.AND.IMOD.NE.0) GO TO 50
C CALL FPRIME(NVAR,X,FPRYM)
C IPEVAL=IPEVAL+1
C DO 10 I=1,NVAR
C   FPRYM(NVAR,I)=0.0
C   FPRYM(NVAR,IP)=1.0
C
C CARRY OUT IN CORE LU DECOMPOSITION OF NVAR BY NVAR MATRIX
C AND USE PIVOT INFORMATION TO COMPUTE DETERMINANT

```


C	CALL SGEFA(FPRYM,NVAR,NVAR,IPUT,INFO)	SLVE0069
	DETA=1.0	SLVE0070
	IEXP=0	SLVE0071
	TWO=2.0	SLVE0072
	DO 40 I=1,NVAR	SLVE0073
	IF (IPUT(I).NE.I) DETA=-DETA	SLVE0074
	DETA=FPRYM(I,I)*DETA	SLVE0075
	IF (DETA.EQ.0.0) GO TO 60	SLVE0076
20	IF (ABS(DETA).GE.1.0) GO TO 30	SLVE0077
	DETA=DETA*TWO	SLVE0078
	IEXP=IEXP+1	SLVE0079
	GO TO 20	SLVE0080
30	IF (ABS(DETA).LT.TWO) GO TO 40	SLVE0081
	DETA=DETA/TWO	SLVE0082
	IEXP=IEXP+1	SLVE0083
	GO TO 30	SLVE0084
40	CONTINUE	SLVE0085
	IF (INFO.NE.0) GO TO 60	SLVE0086
C		SLVE0087
C	USING L-U FACTORED MATRIX, SOLVE SYSTEM USING FORWARD-BACKWARD	SLVE0088
C	ELIMINATION, AND OVERWRITE RIGHT HAND SIDE WITH SOLUTION	SLVE0089
C		SLVE0090
	50 CALL SGESL(FPRYM,NVAR,NVAR,IPUT,Y,0)	SLVE0091
	IERR=0	SLVE0092
	RETURN	SLVE0093
60	IERR=1	SLVE0094
	INFO=0	SLVE0095
	RETURN	SLVE0096
C		SLVE0097
C	*****	SLVE0098
C		SLVE0099
	END	SLVE0100
		SLVE0101

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